Output Error Estimates and Mesh Refinement in Aerodynamic Shape Optimization

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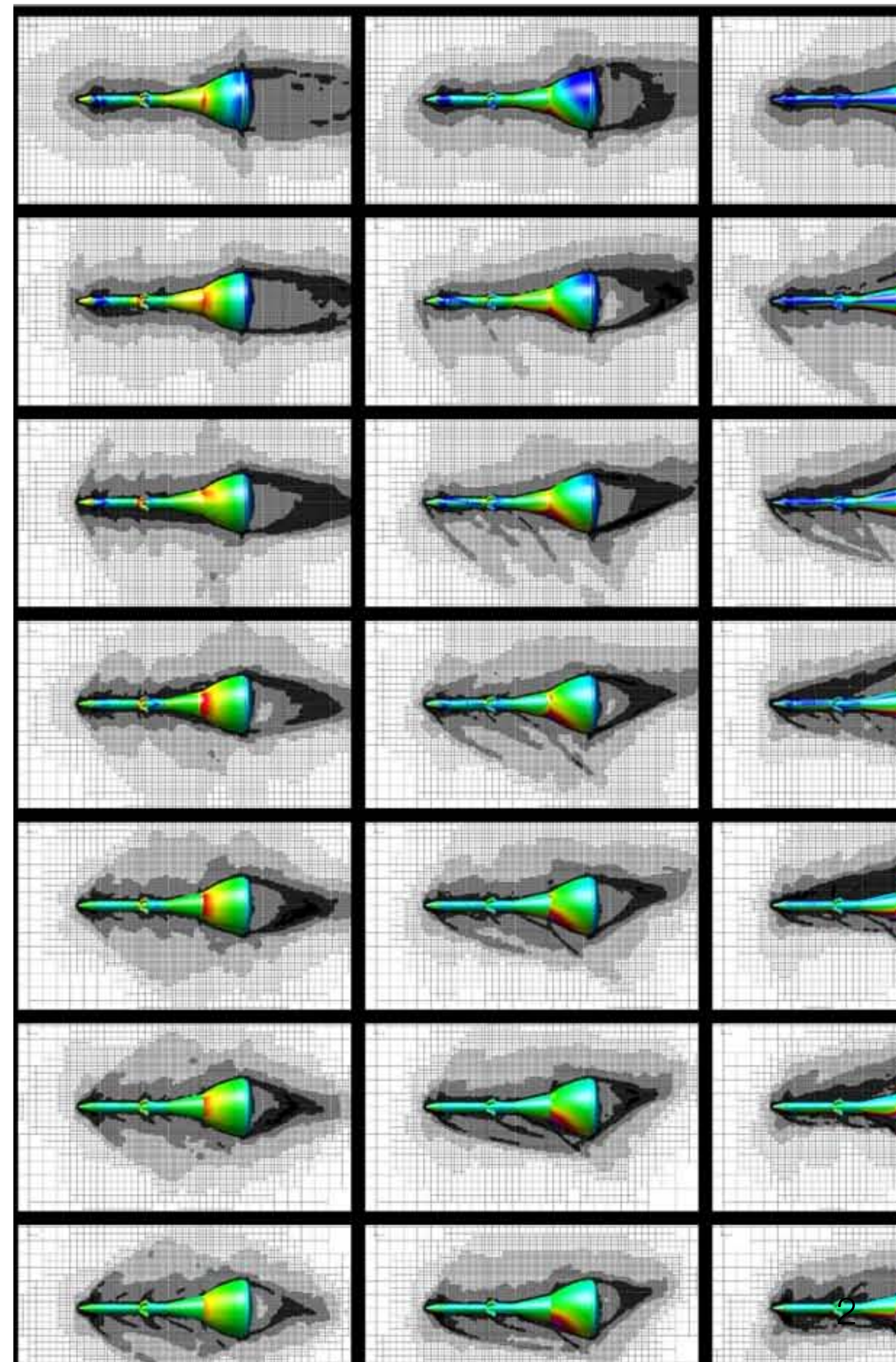
AIAA Paper 2013-0865
51st AIAA Aerospace Sciences Meeting
January 9, 2013

Motivation

- Success of output error estimation and adaptive mesh refinement in goal-oriented simulations
  - Automatic and user-independent production databases
- Challenges of simulation-based design
  - High CFD expertise
    - Reliable mesh generation, long setup time
    - High cost due to repeated evaluation of objectives on fine, hand-crafted meshes or high uncertainty due to inappropriate meshes



Objectives

Adaptive discretization of aerodynamic shape optimization problems

Accuracy

- Improve design confidence
  - Direct control over objective function discretization error

Automation

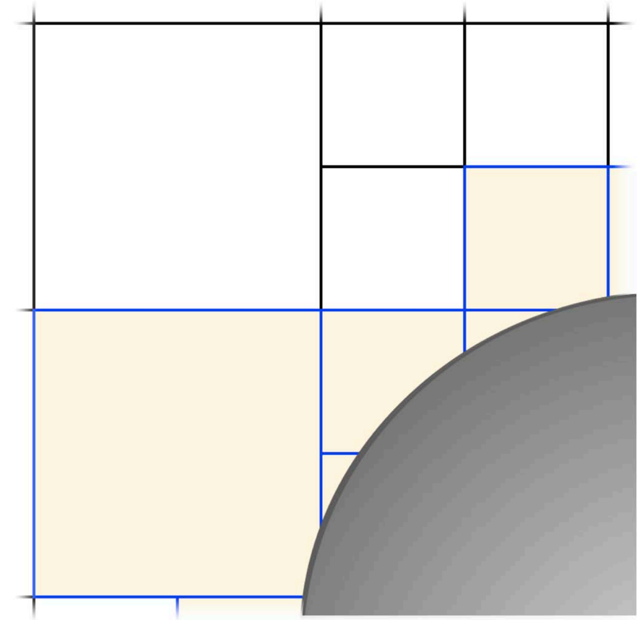
- Reduce level of CFD expertise
  - Eliminate the requirement to hand-craft general meshes appropriate for all candidate designs
  - Shorten problem setup time

Progress toward improved efficiency

- Reduce cost by systematically increasing the depth of refinement as the design improves
  - Progressive optimization strategy
  - Investigate challenges of dynamic error control

Previous Work - Infrastructure

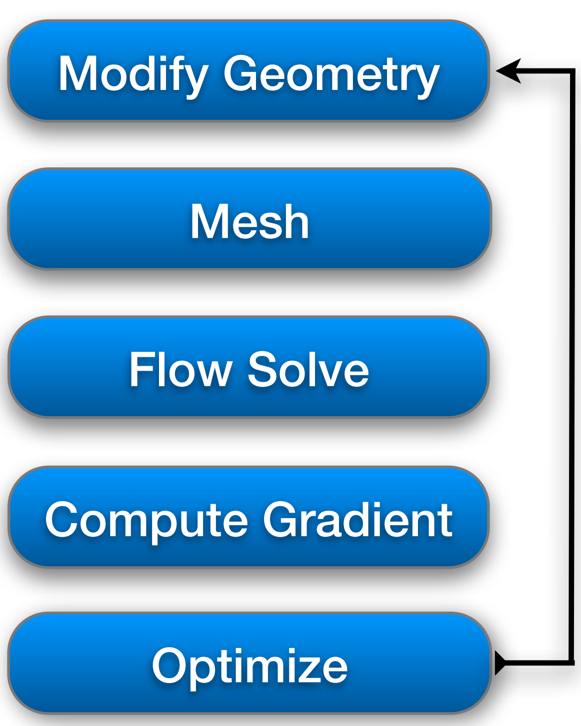
1. Embedded-boundary Cartesian mesh method
   - Arbitrarily complex domains, efficient and accurate
   - Irregularity confined to body intersecting cells



2. Incremental strategy for h-refinement

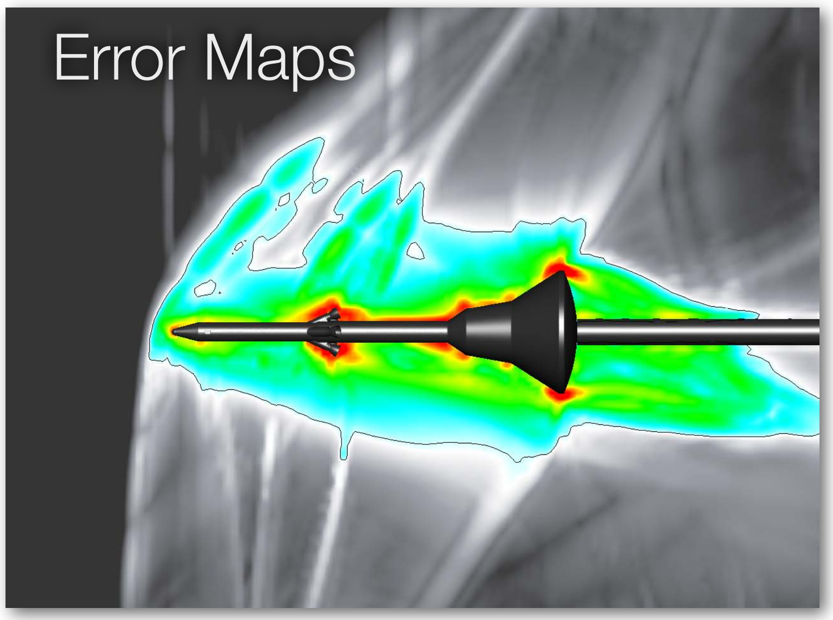
Adjoints

3. Aerodynamic shape optimization
   - Gradient computation

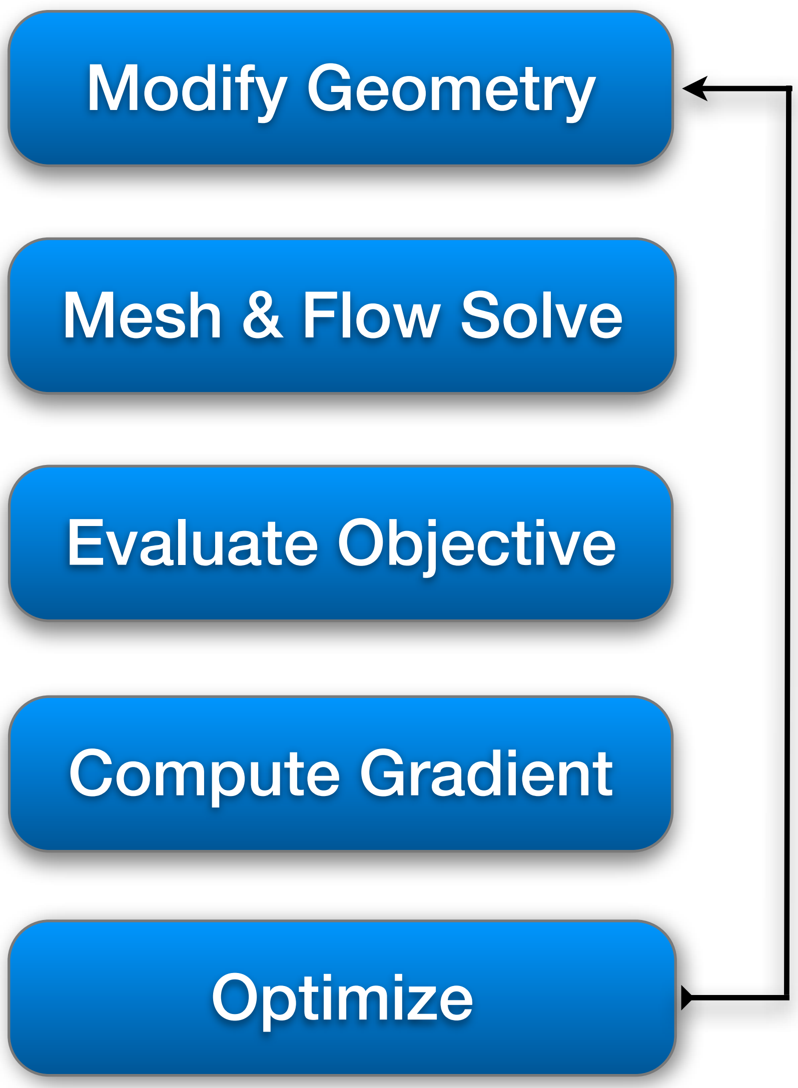


See AIAA Paper 2013-0543 (Smith et al.) for applications

4. Output error estimates
   - Adaptive mesh refinement



Optimization: Discrete Formulation



$$\min_{X} \quad J\left(X, \mathbf{Q}\right)$$

subject to

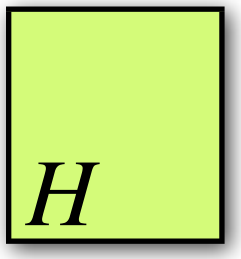
$$R\left(X, \mathbf{Q}\right) = 0 \qquad \forall X \in \Omega$$

- Steady Euler equations
- Gradient-based optimization $\dfrac{\mathrm{d}J}{\mathrm{d}X}$
  - BFGS
  - SNOPT
- Shape optimization

$$\mathbf{M} = f[\mathbf{T}(X)]$$

Role of Adjoints

Gradients



$$J = f(X, \mathbf{Q})$$

e.g. $C_D + (C_L - C_L^*)^2$

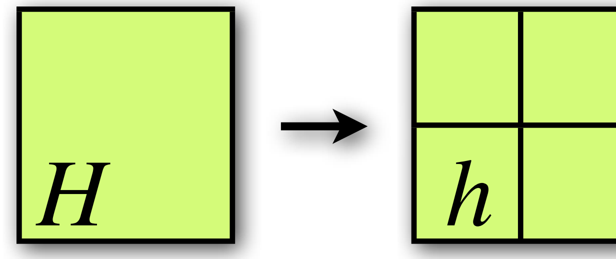
$$\frac{\mathrm{d}J}{\mathrm{d}X} = \frac{\partial J}{\partial X} + \frac{\partial J}{\partial \mathbf{Q}} \frac{\mathrm{d}\mathbf{Q}}{\mathrm{d}X}$$

$$0 = \frac{\partial \mathbf{R}}{\partial X} + \frac{\partial \mathbf{R}}{\partial \mathbf{Q}} \frac{\mathrm{d}\mathbf{Q}}{\mathrm{d}X}$$

$$\frac{\mathrm{d}J}{\mathrm{d}X} = \frac{\partial J}{\partial X} - \psi^{\mathrm{T}} \frac{\partial \mathbf{R}}{\partial X}$$

$$\boxed{\left[\frac{\partial \mathbf{R}}{\partial \mathbf{Q}}\right]^{\mathrm{T}} \psi = \frac{\partial J}{\partial \mathbf{Q}}}$$

Error Estimates



$$e = |J_h - J_H)|$$

$$J_h \approx J_h(\mathbf{Q}_H) + \frac{\partial J(\mathbf{Q}_H)}{\partial \mathbf{Q}} \Delta \mathbf{Q}$$

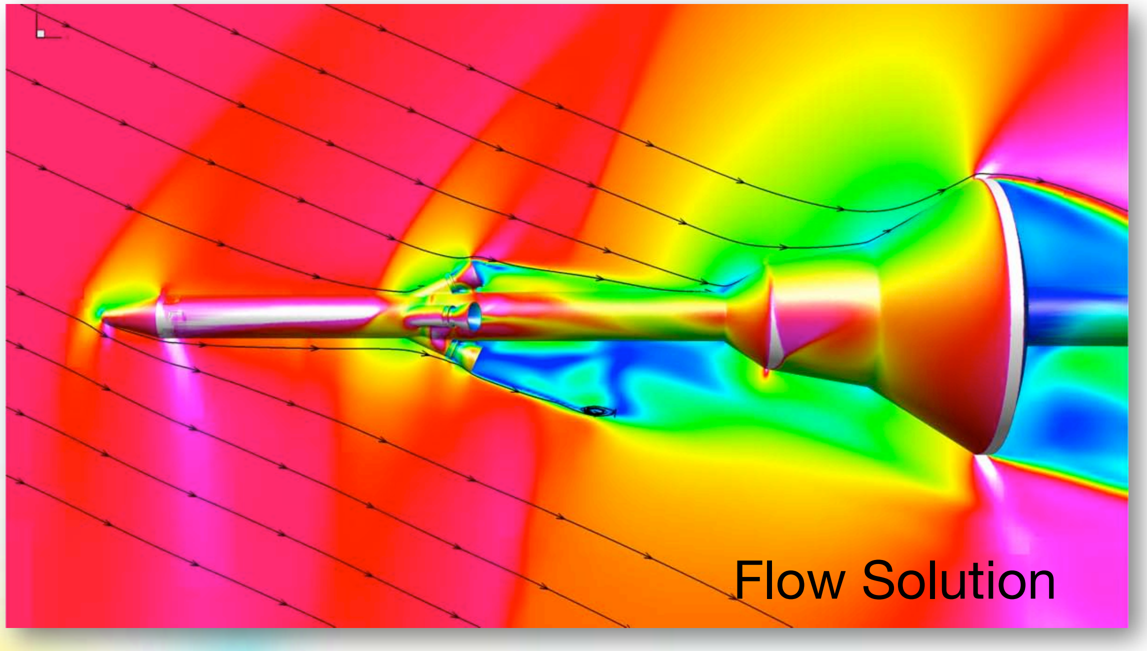
$$0 \approx R_h(\mathbf{Q}_H) + \frac{\partial R(\mathbf{Q}_H)}{\partial \mathbf{Q}} \Delta \mathbf{Q}$$

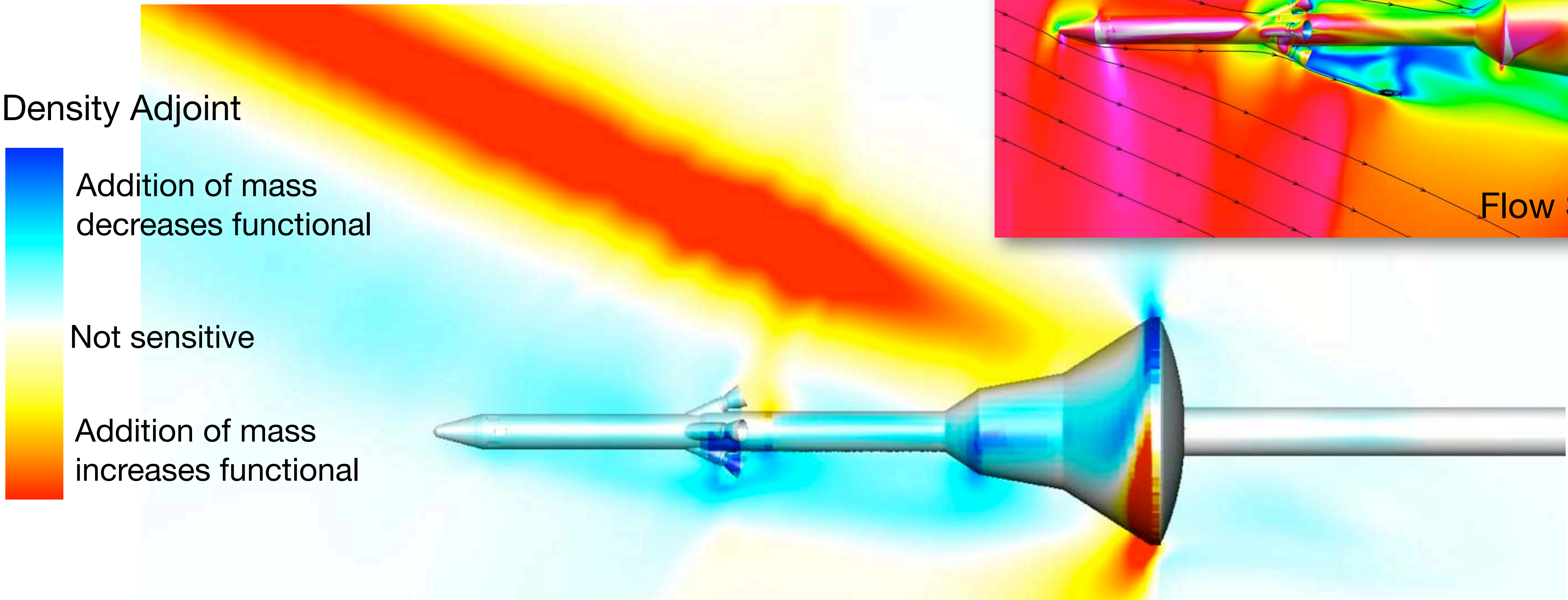
$$J_h \approx J_h(\mathbf{Q}_H) - \psi^{\mathrm{T}} \mathbf{R}_h(\mathbf{Q}_H)$$

Role of Adjoints

M_∞=1.1, α=-25°

$$J = C_N + 0.2C_A$$





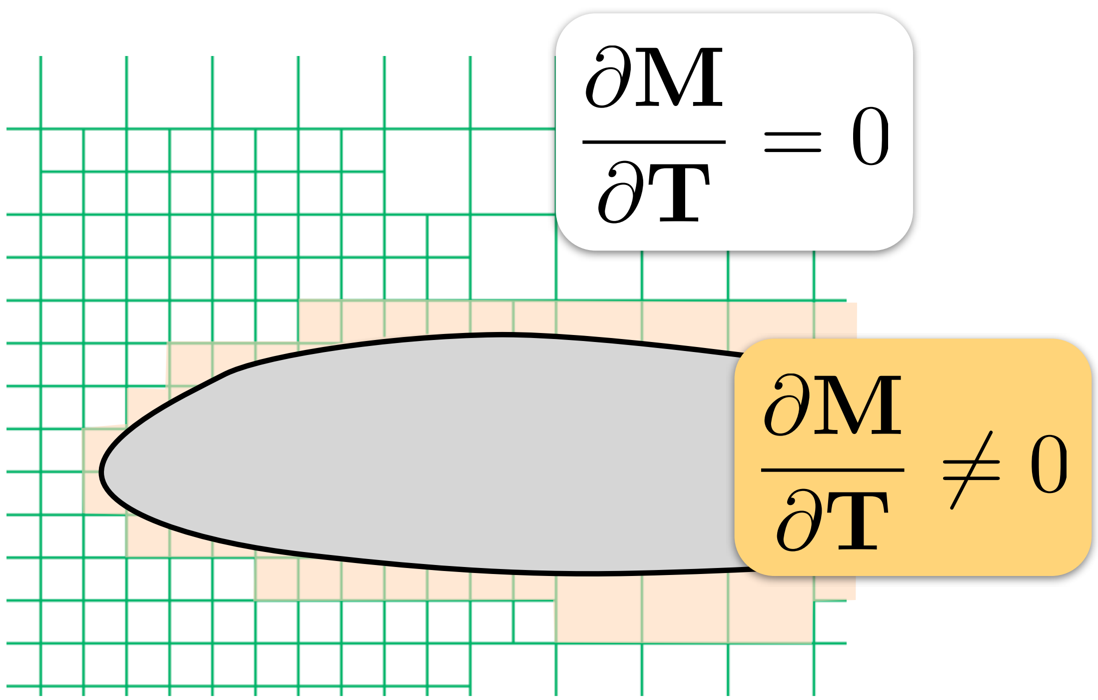
- Control problem
  - Optimal shape design: adjust design variables to control the flow and improve performance
  - Error analysis: adjust mesh refinement to control discretization errors

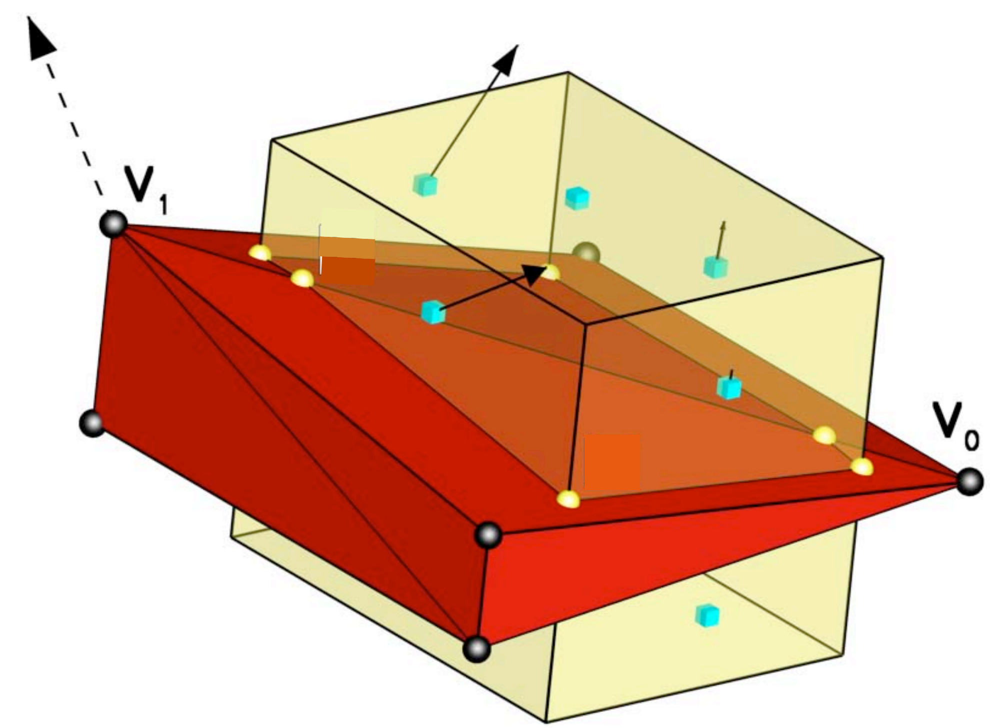
Linearization Details

- Objective function gradient

$$\frac{\mathrm{d}\mathcal{J}}{\mathrm{d}X} = \frac{\partial \mathcal{J}}{\partial X} + \frac{\partial \mathcal{J}}{\partial \mathbf{M}} \frac{\partial \mathbf{M}}{\partial \mathbf{T}} \frac{\partial \mathbf{T}}{\partial X} - \psi^{\mathrm{T}} \left(\frac{\partial \mathbf{R}}{\partial X} + \frac{\partial \mathbf{R}}{\partial \mathbf{M}} \frac{\partial \mathbf{M}}{\partial \mathbf{T}} \frac{\partial \mathbf{T}}{\partial X} \right)$$

- Mesh sensitivities: infinitesimal perturbations are confined to cutcells





- Triangle to cut-cell connectivity established on-the-fly as the design evolves: triangulation connectivity and topology allowed to change

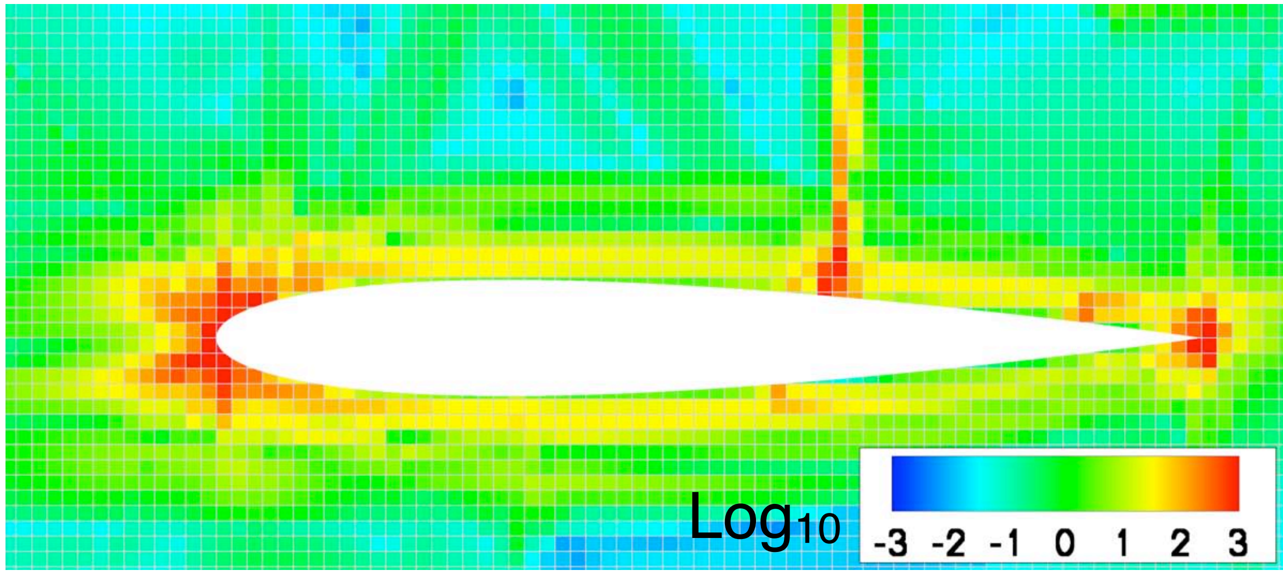
Error-Estimate Details

$$J(\mathbf{Q}_h) \approx J(\mathbf{Q}_h^H) - (\psi_h^H)^{\mathrm{T}}\mathbf{R}(\mathbf{Q}_h^H) - (\psi_h - \psi_h^H)^{\mathrm{T}}\mathbf{R}(\mathbf{Q}_h^H)$$

Remaining Error

- Bound on remaining error in each coarse cell k

$$e_k = \sum_{i=1}^{5} \left| (\psi_{\mathrm{Q}} - \psi_{\mathrm{L}})^{\mathrm{T}} \mathbf{R}(\mathbf{Q}_{\mathrm{L}}) \right|_i$$

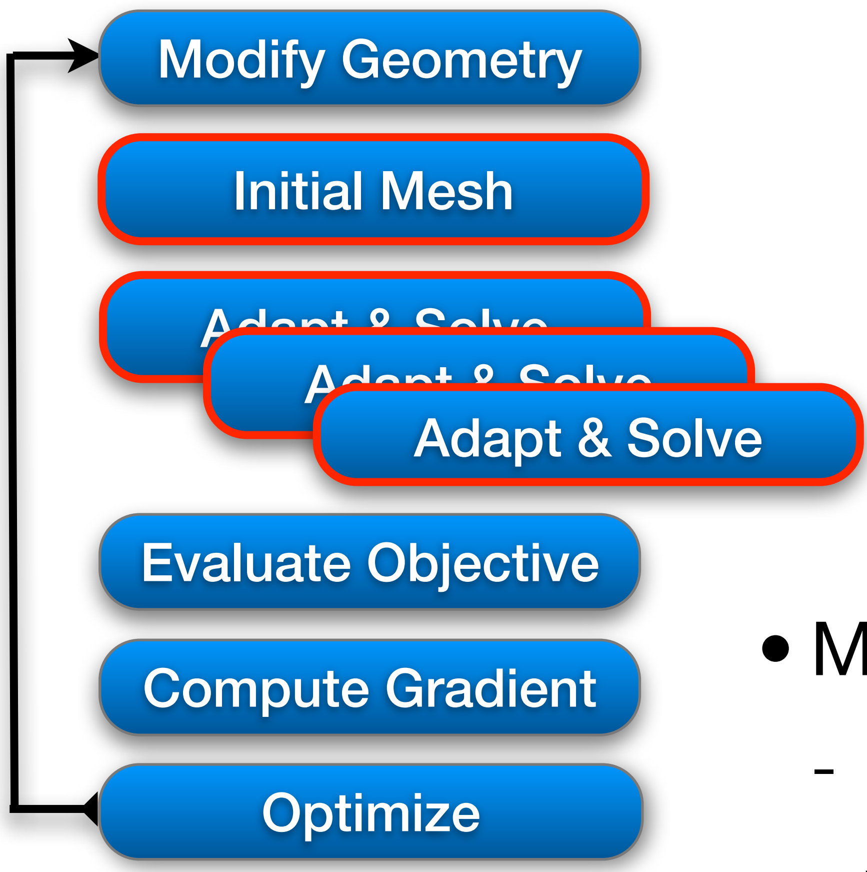


- Net functional error $\quad E = \sum_{k=0}^{N} e_k$

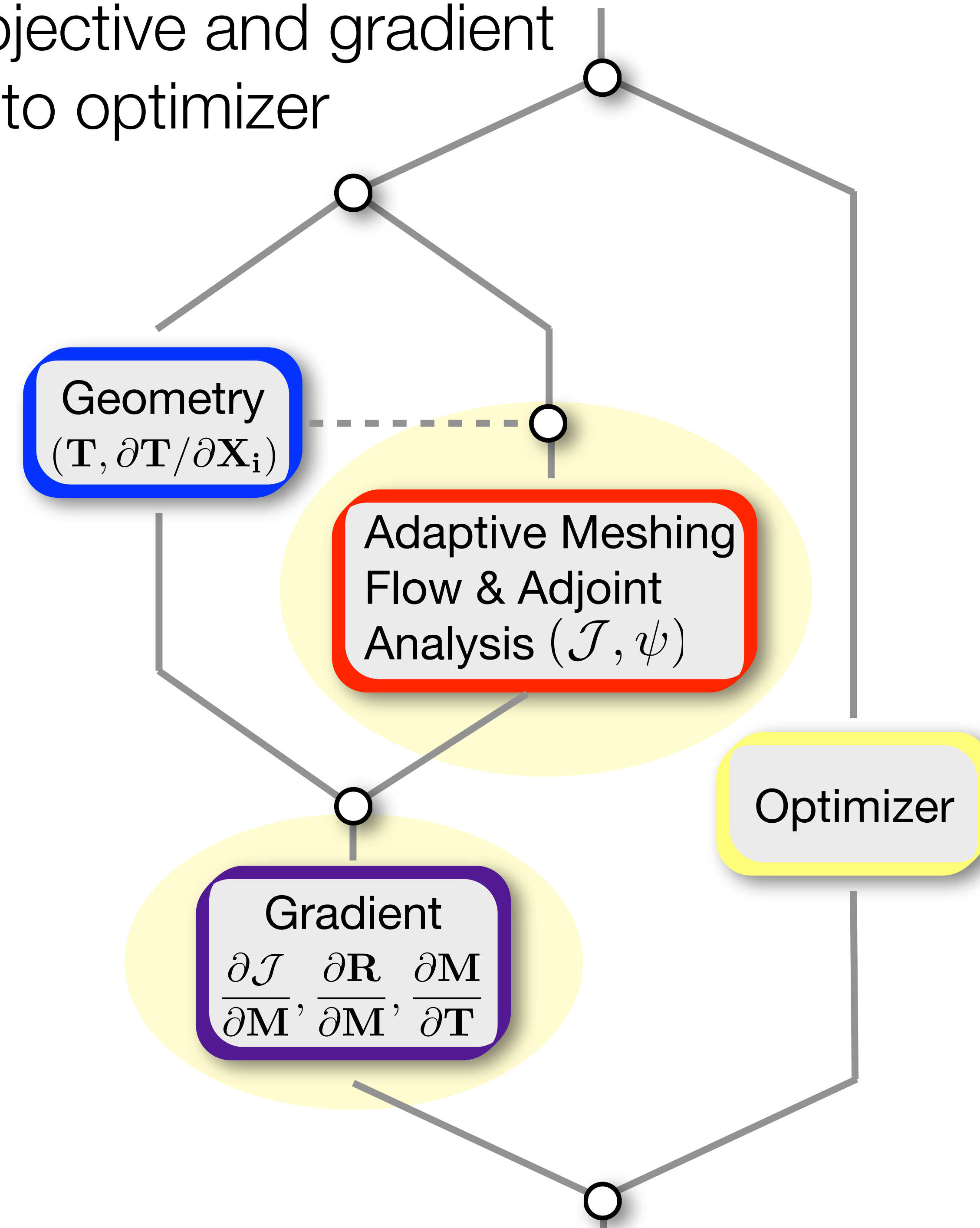
- Given a user specified tolerance TOL, refine until E < TOL

- In practice, specify number of cycles, mesh-growth factor per cycle and cell-budget

Basic Framework Integration

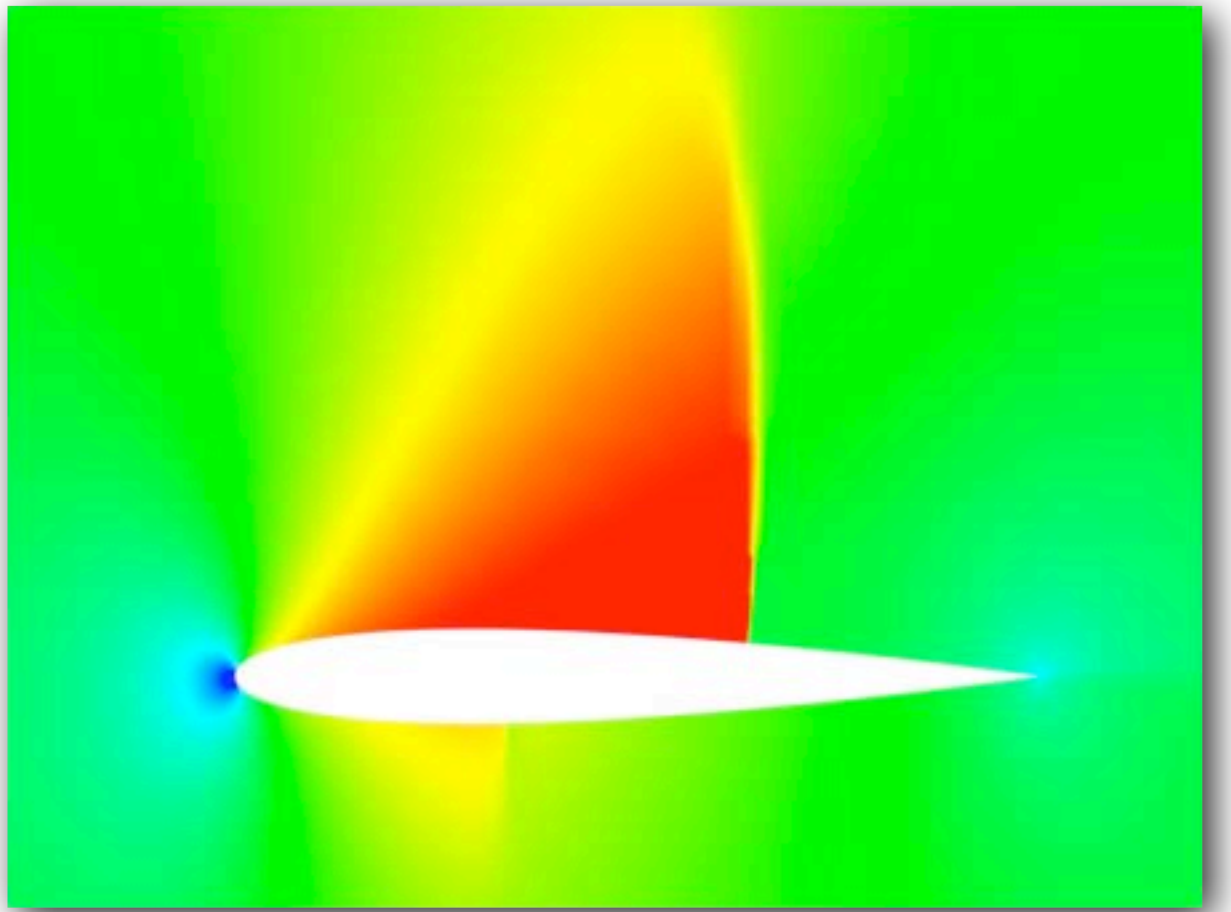


- Integration into existing, fixed mesh, optimization framework
  - Build sequence of adapted meshes
  - Pass values of objective and gradient from finest mesh to optimizer
- Multilevel parallelism
  - Mesh sensitivities in stand-alone code
- In each design iteration, perform fixed (user specified) number of adaptations
  - Fixed depth strategy
  - Very robust and precise control over computational resources
  - May be inefficient



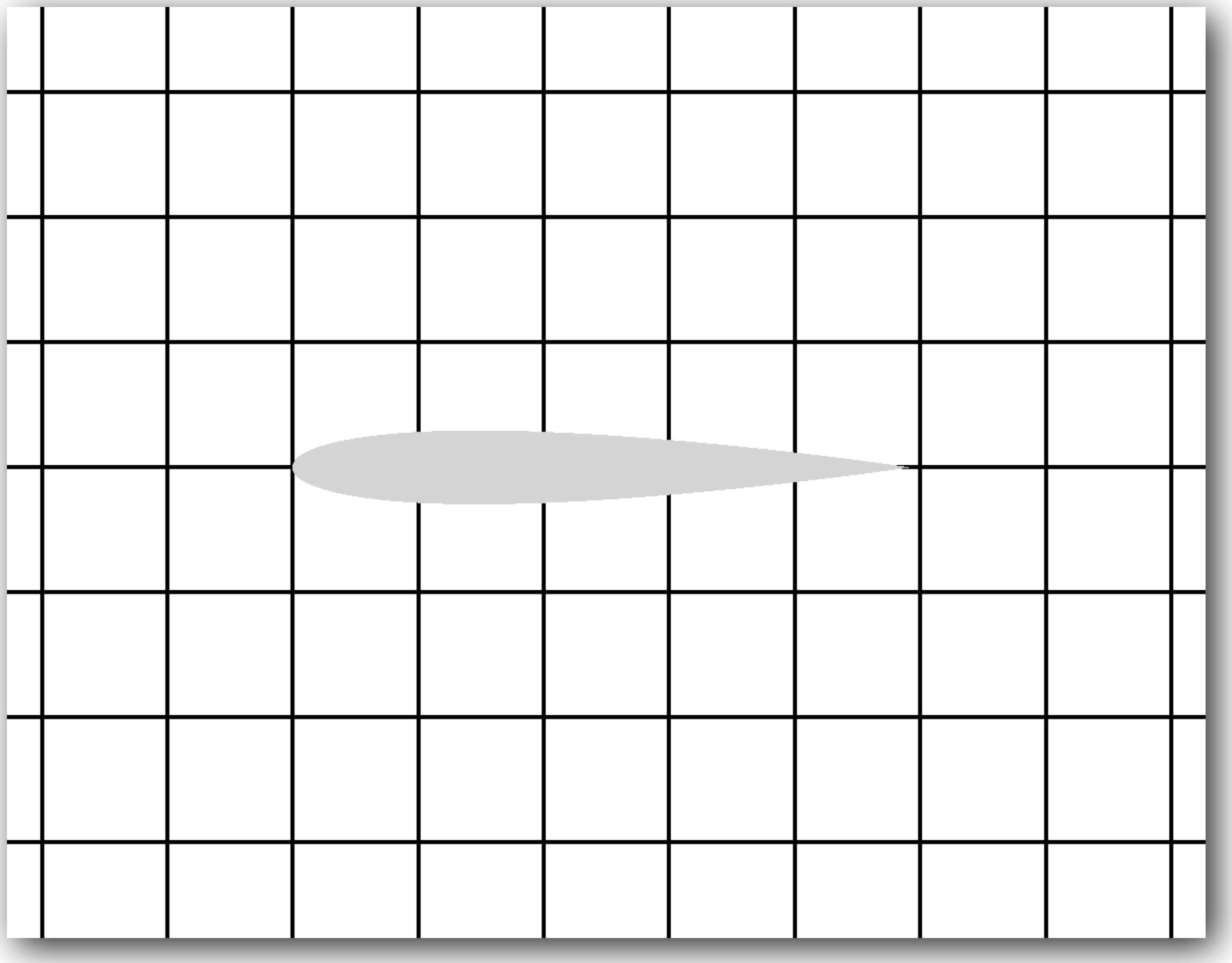
Basic Example

- Demonstrate numerical optimization with adaptive meshing
- Study mesh convergence of objective function, its error estimates and gradients
- Find angle of attack to minimize drag coefficient
  - Transonic flow, $M_\infty = 0.8$
  - NACA 0012 airfoil
  - $J = C_d$, $X = \alpha$
  - Initial design: $\alpha_i = 2°$



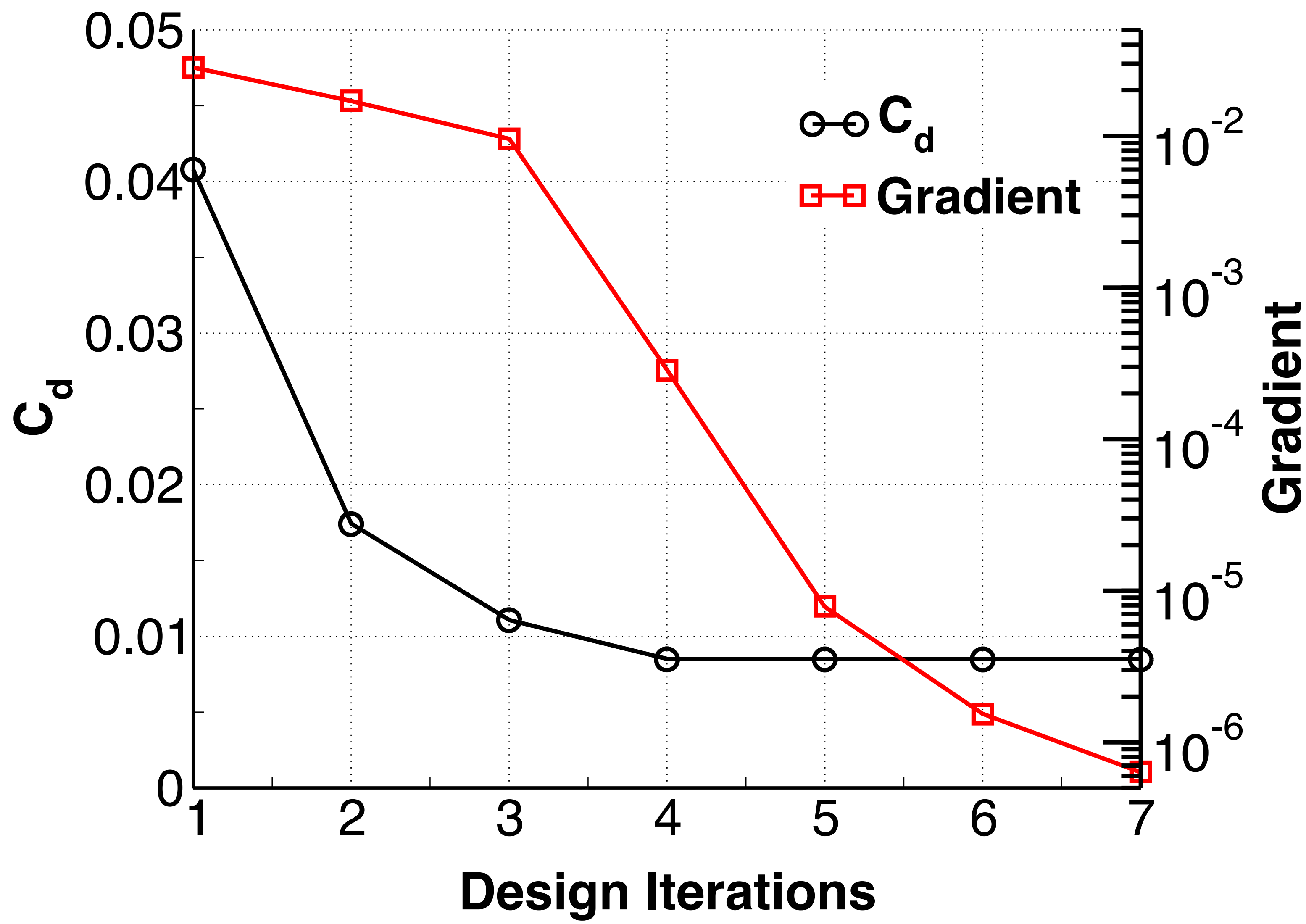
Mesh Setup

- Demonstrate numerical optimization with adaptive meshing
- Study mesh convergence of objective function, its error estimates and gradients
- Fixed-depth strategy
  - 8 adaptive refinements at each design iteration
  - Initial mesh ~1,700 cells
  - Final mesh ~25,000 cells



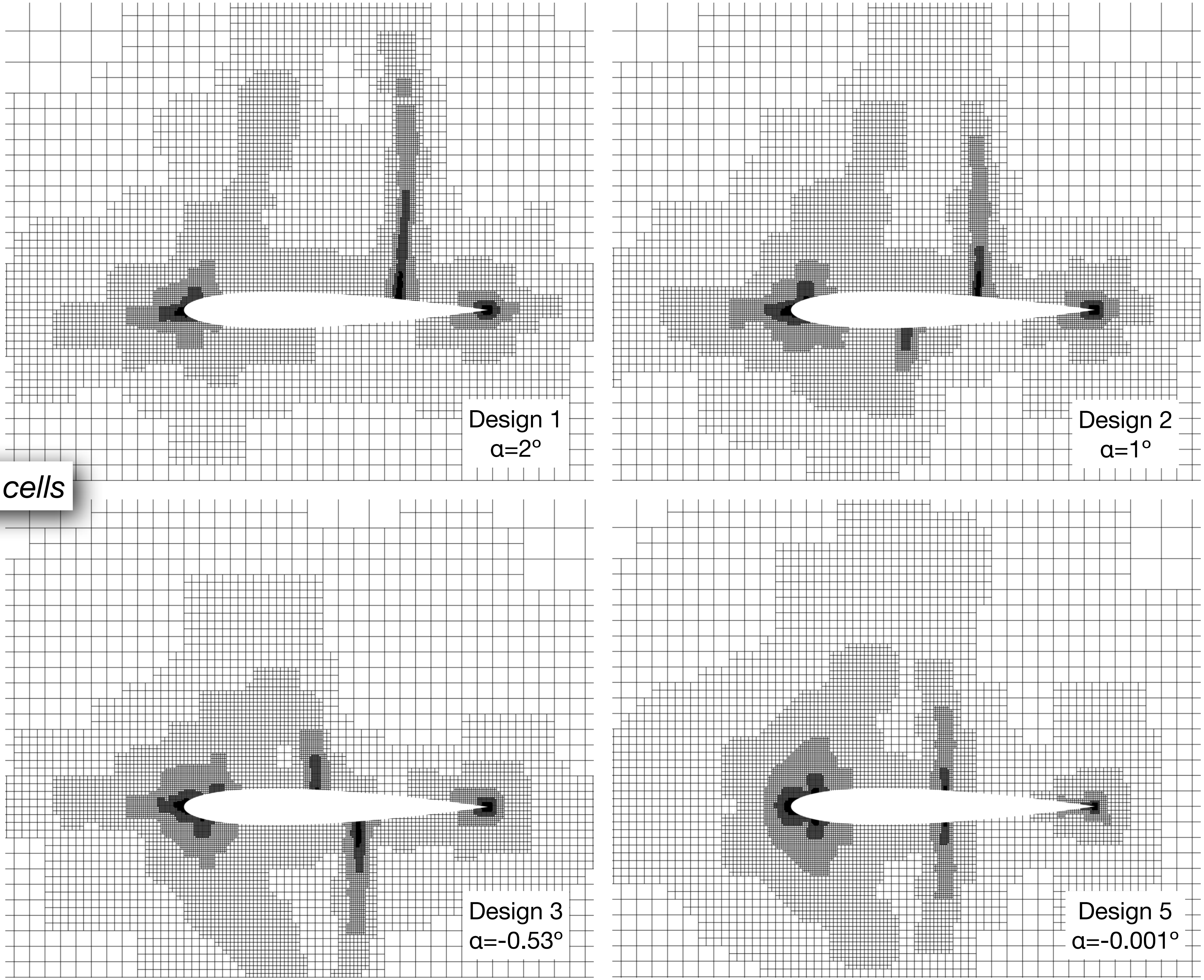
Near-field view of initial mesh

Optimization Convergence History



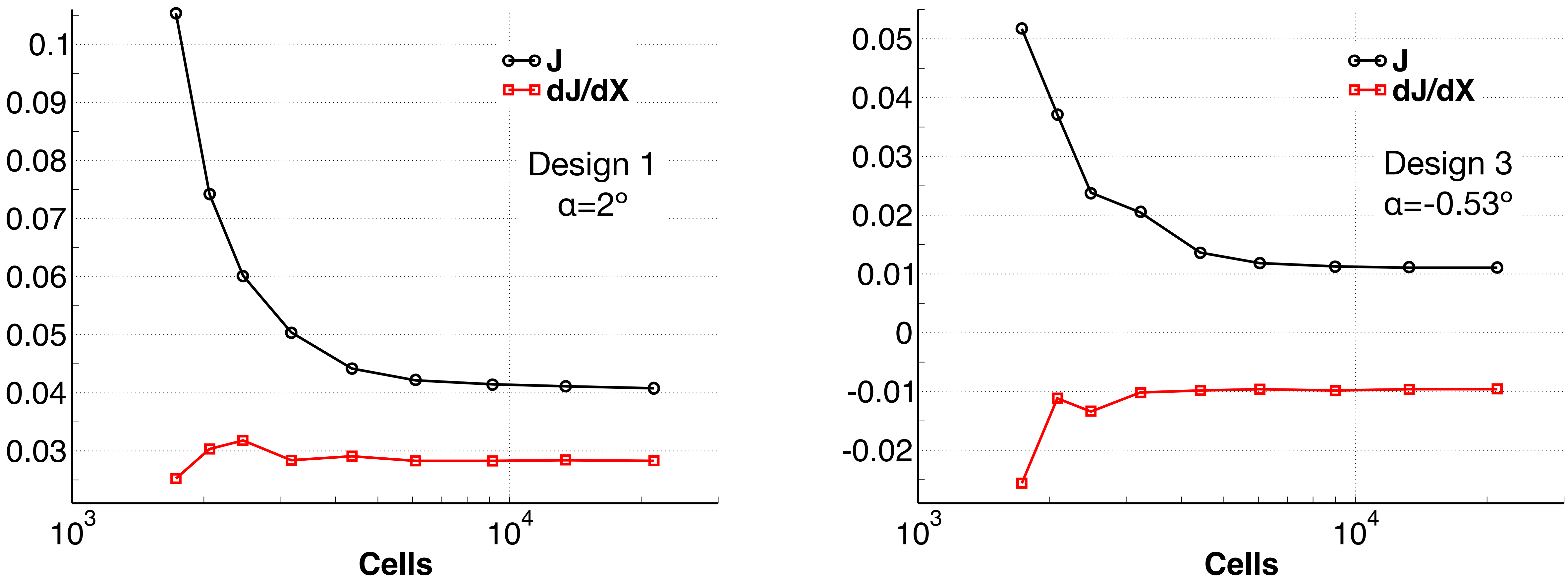
- Optimizer minimizes drag in 7 iterations
- Gradient reduced by almost 5 orders of magnitude
- Angle of attack history: 2°, 1°, -0.5°, 0.01°, -0.001°

Final Meshes After 8 Adaptations



~25,000 cells

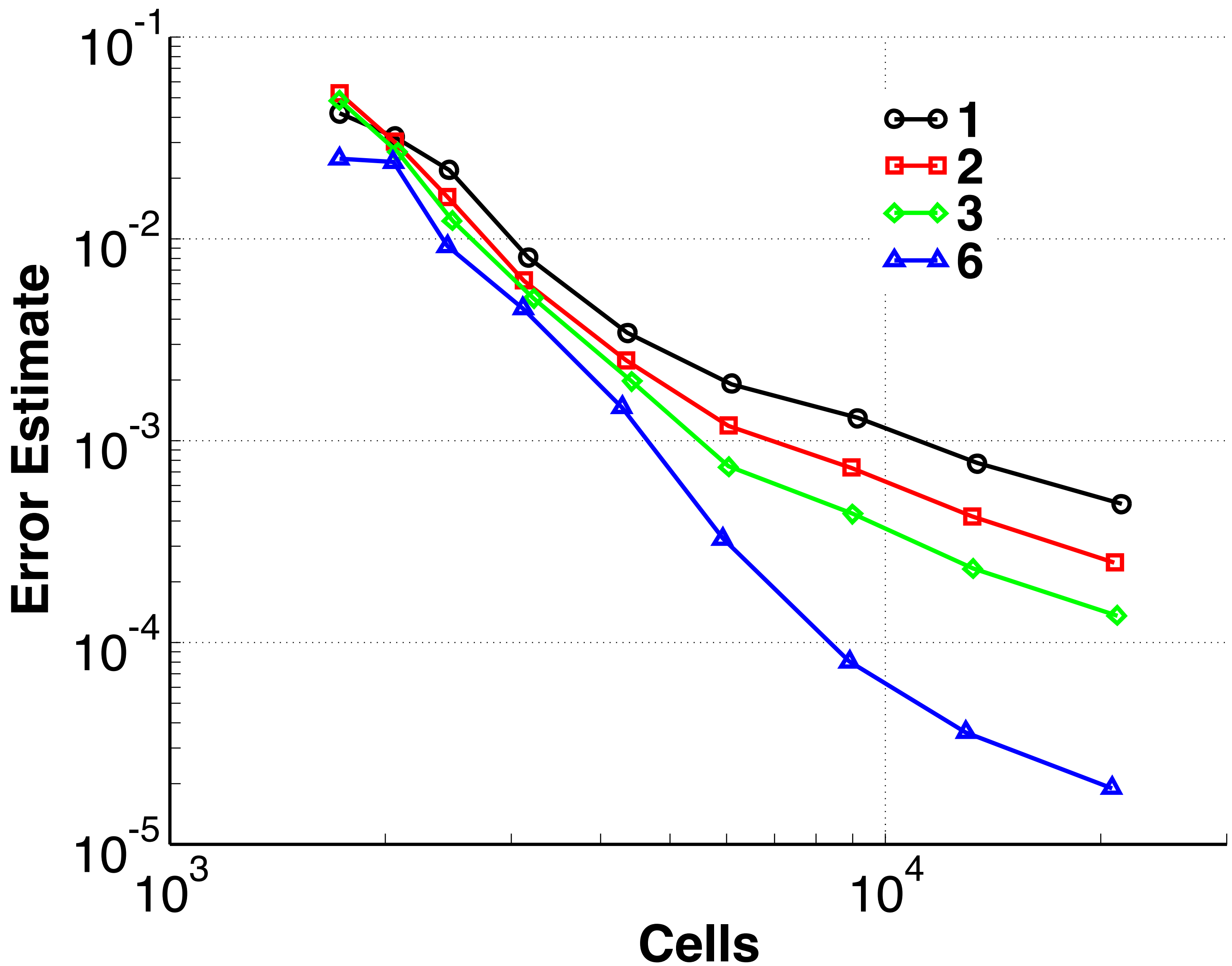
Output Mesh Convergence



Mesh convergence of drag and gradient at selected design iterations

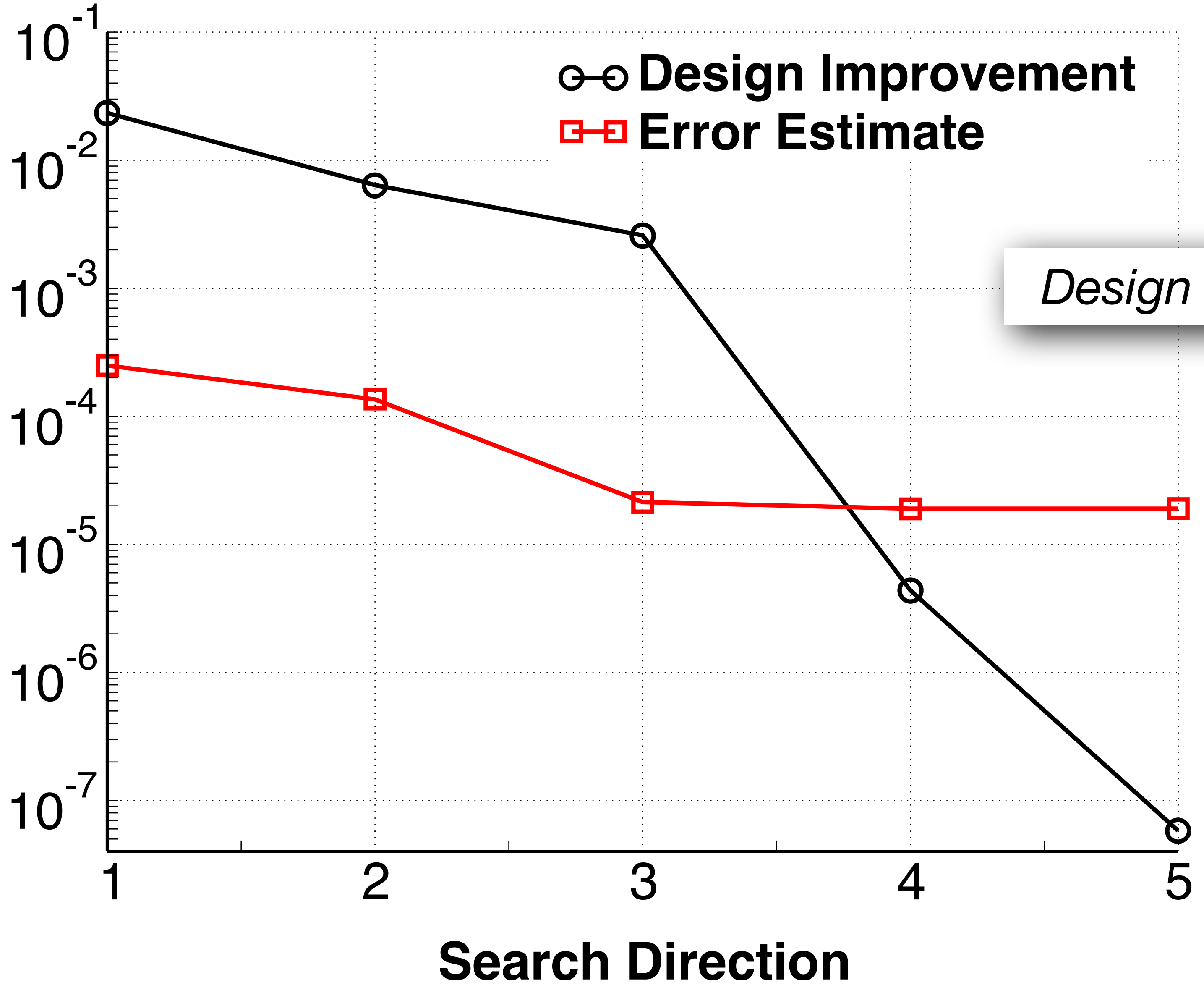
- Drag and gradient are well converged on meshes with ~10,000 cells
- Sign predicted correctly even on the coarsest mesh

Convergence of Error Estimates



- Key parameter to safeguard oversolving and transfer optimization to next mesh

Mesh Efficiency of Fixed-Depth Strategy



Design Improvement $= J_{i-1} - J_i$

Mesh too fine — *Mesh too coarse*

- Angle of attack history: 2°, 1°, -0.5°, 0.01°, -0.001°

Objectives in Quadratic Form

- Frequently use objective functions that contain quadratic terms
  - Penalty terms, e.g. $(C_L - T)^2$
  - Inverse design, e.g. $J = \int (P - P_{\text{target}})^2 dS$

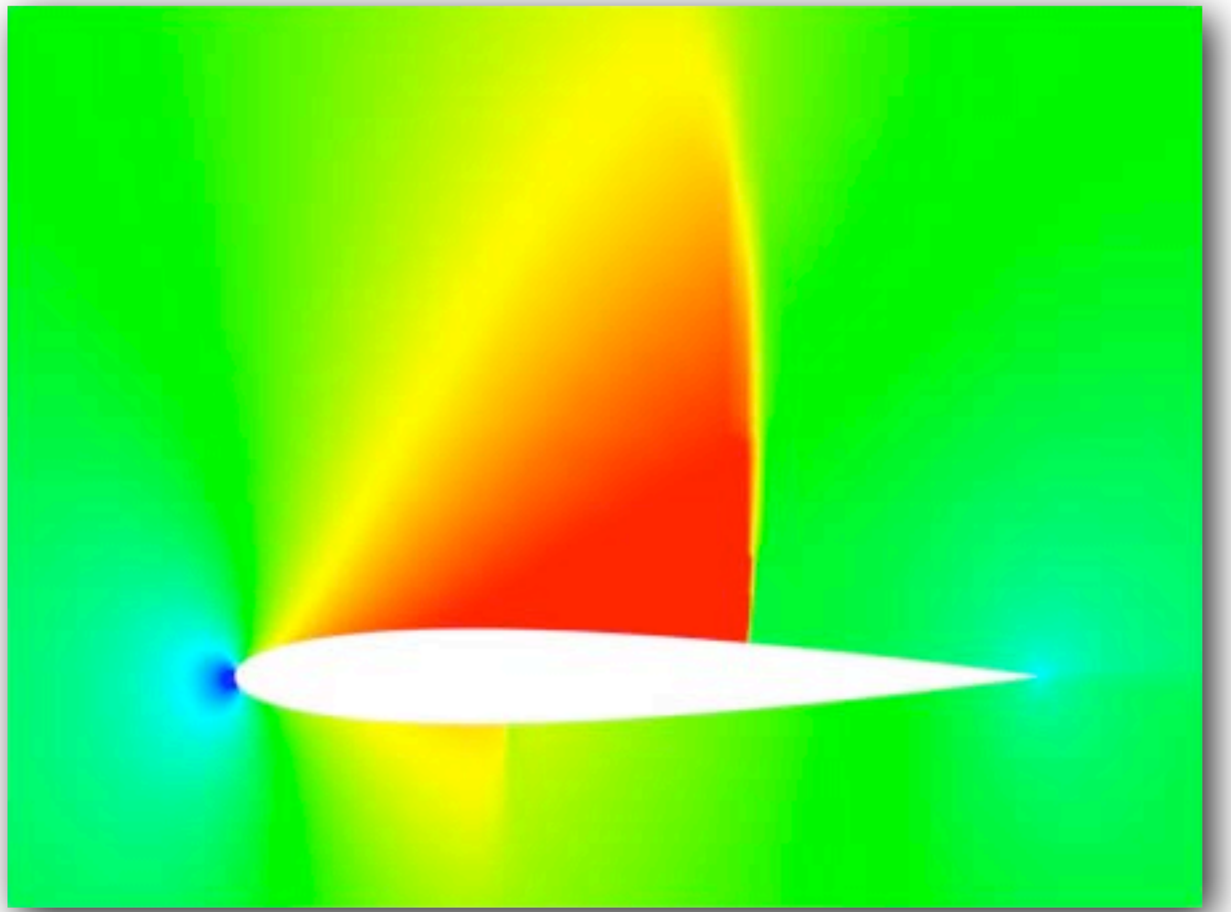
- As working variable approaches its target, adjoint variables vanish

$$\left[\frac{\partial \mathbf{R}}{\partial \mathbf{Q}}\right]^{\mathrm{T}} \psi = \frac{\partial \mathcal{J}}{\partial \mathbf{Q}}^{\mathrm{T}} \longrightarrow \frac{\partial \mathcal{J}}{\partial Q} = 2(\overset{0}{\cancel{P - T}})\frac{\partial P}{\partial Q}$$

- Consequences include vanishing error estimates as optimality is approached, which effectively terminate adaptation, as well as strongly non-monotone error convergence

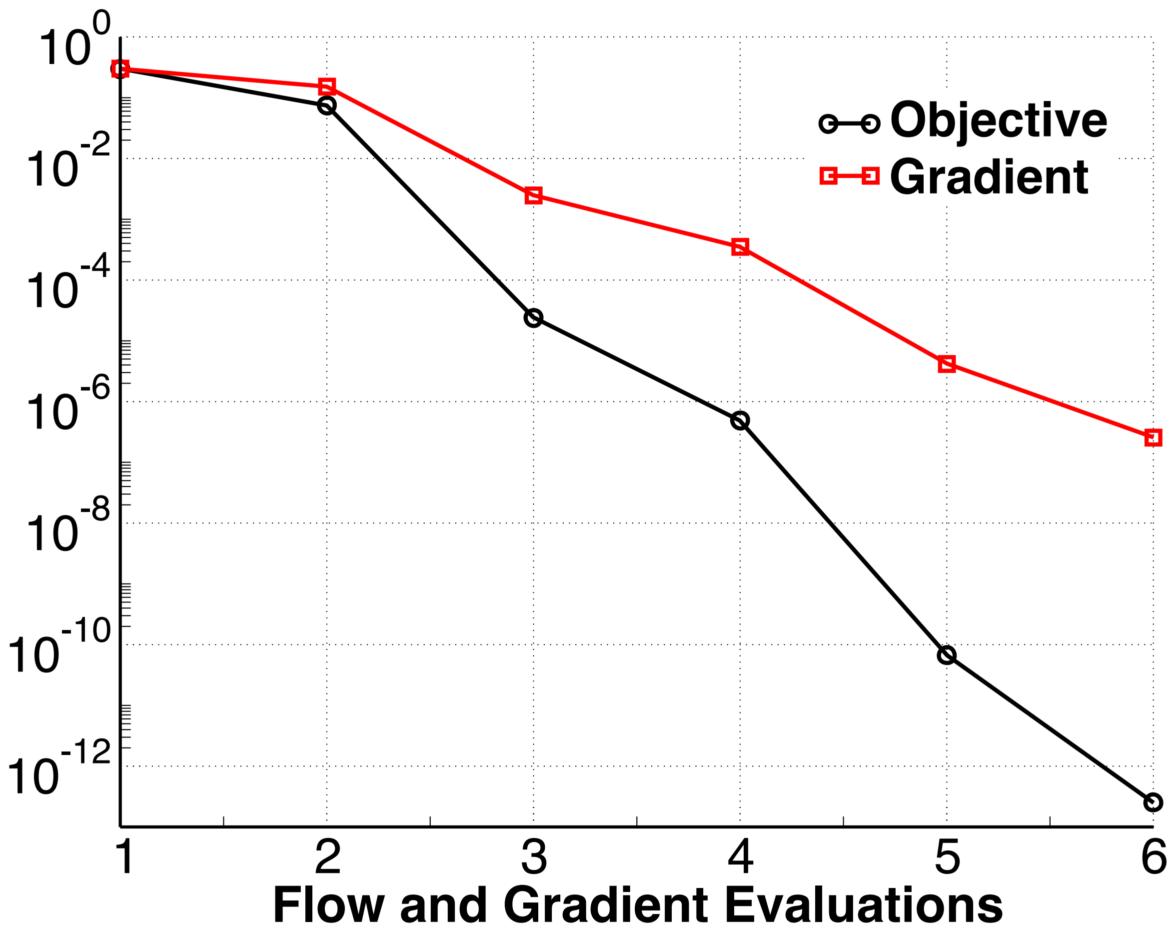
Quadratic Example

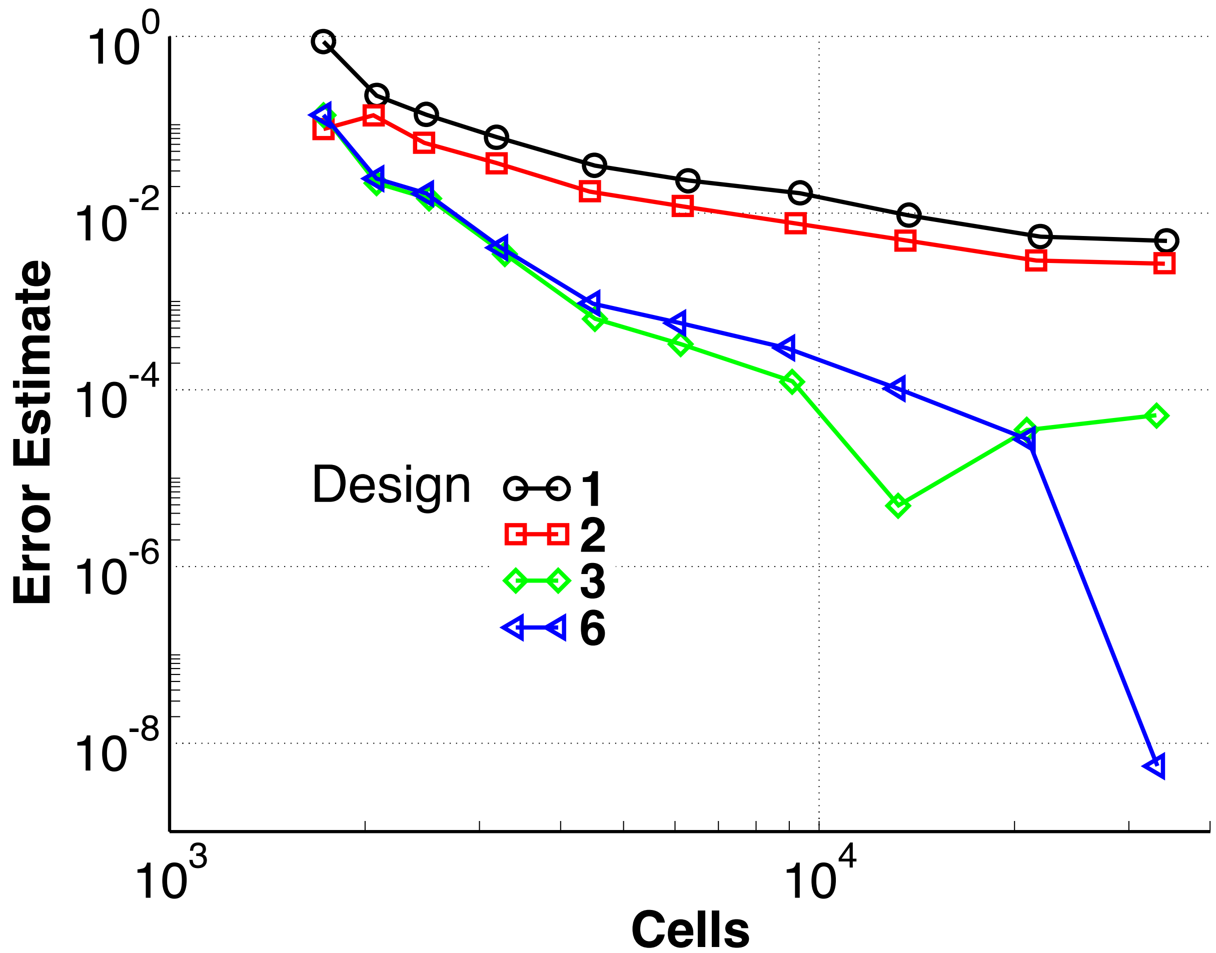
- Find angle of attack to match a target lift coefficient
  - Transonic flow, $M_\infty = 0.8$
  - NACA 0012 airfoil
  - $J = (C_l - 0.55)^2$, $X = \alpha$
  - Initial design: $\alpha_i = 0°$
  - Final design: $\alpha_f \approx 2°$



- Fixed-depth strategy
  - 9 adaptive refinements at each design iteration
  - Initial mesh ~1,700 cells; final mesh ~35,000 cells

Convergence Histories





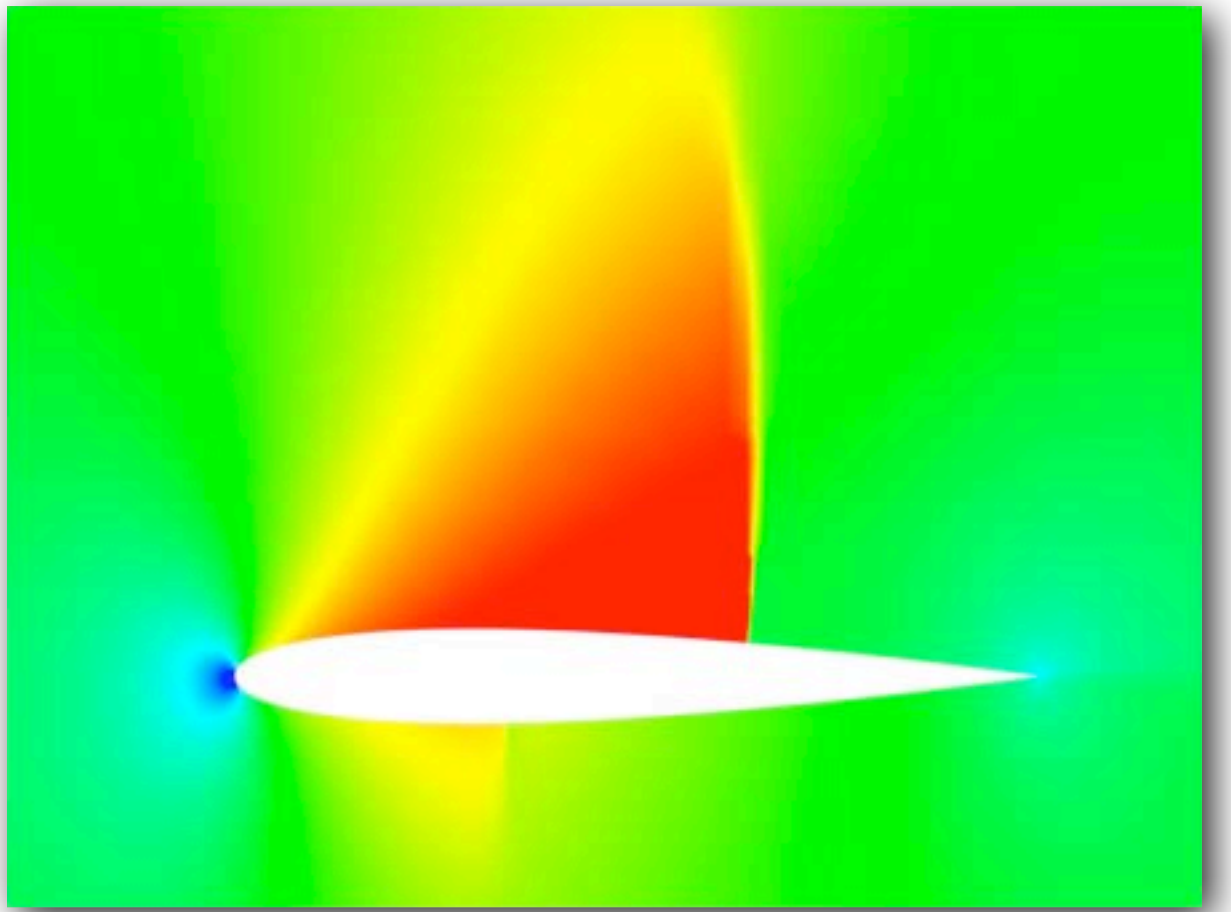
- Optimizer matches lift in 6 iterations
- Error convergence satisfactory in early design iterations, but becomes non-monotone and errors vanish at optimality

"Companion" Functional

- Use a companion functional to eliminate numerical artifacts for quadratic objectives
    - Objective function working variable is used for error control and drives adaptation
    - Objective function drives design
- Possible to implement at no additional cost
    - Arrange computations to use error estimates from the penultimate adaptation cycle and solve objective function adjoint only on the finest mesh

Quadratic Example

- Find angle of attack to match a target lift coefficient
  - $J = (C_l - 0.55)^2$, $X = \alpha$
  - $J_{EC} = C_l$, Error Estimate = ε



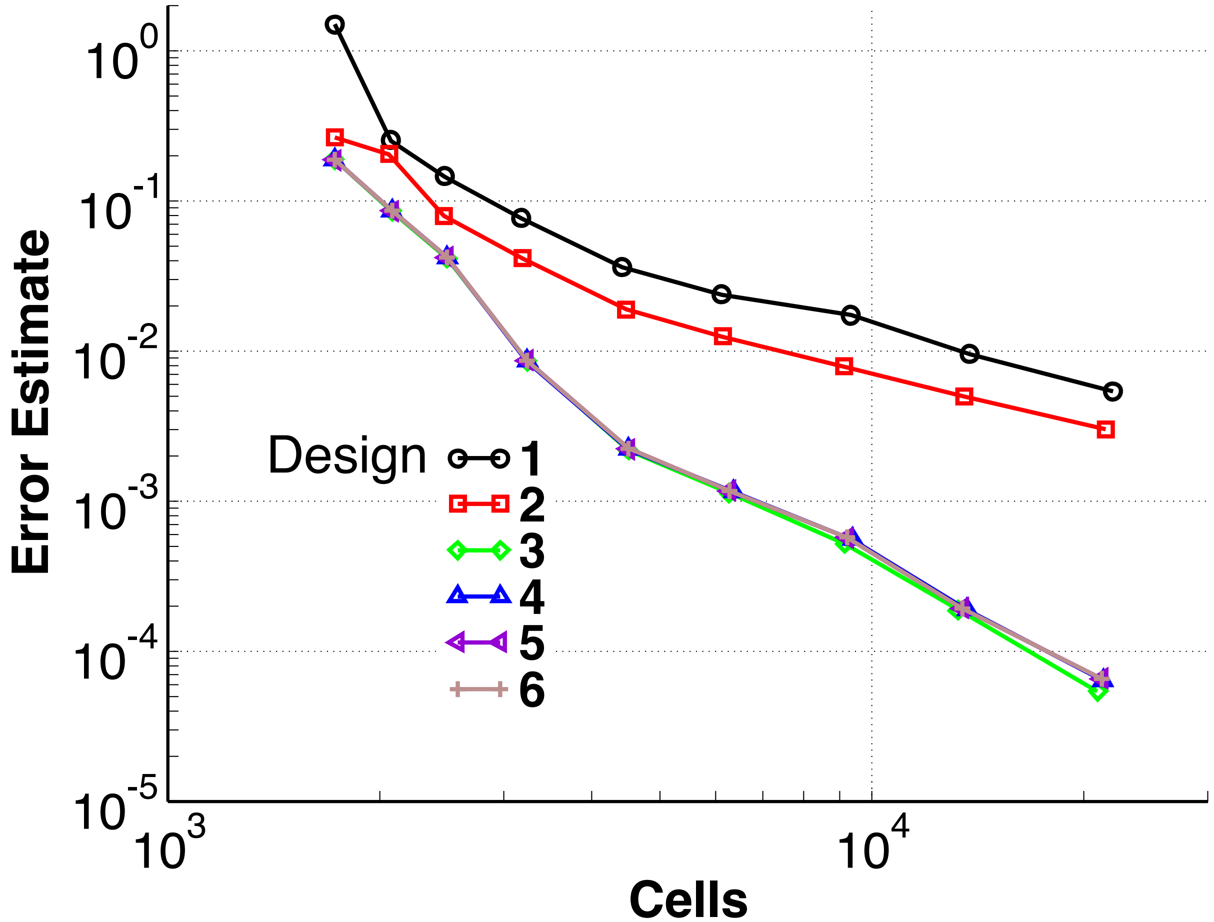
- Compute conservative error estimate in objective function

$$J = ((C_l \pm \varepsilon) - 0.55)^2$$

$$J \leq (C_l - 0.55)^2 \pm \Delta$$

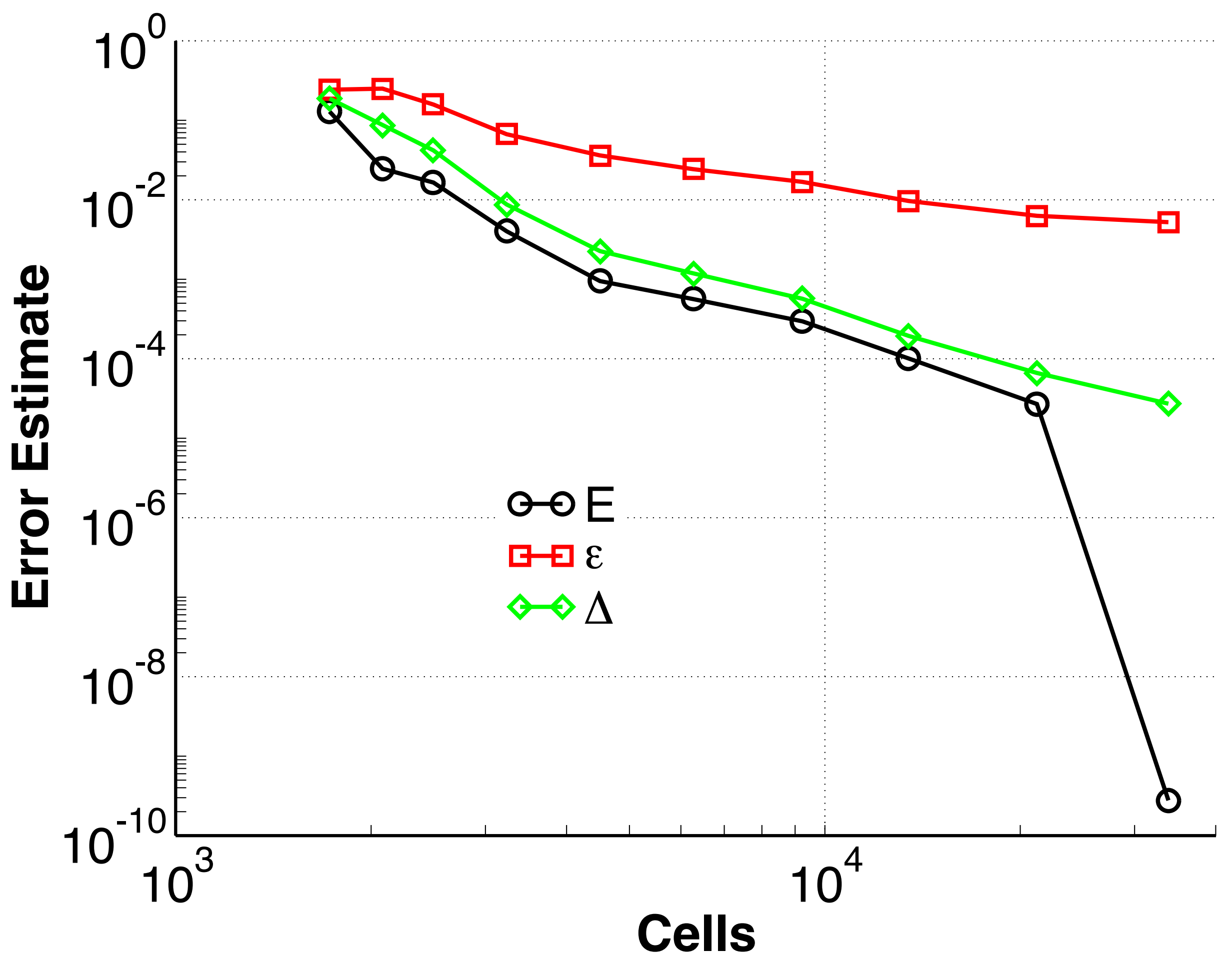
$$\Delta = |2(C_l - 0.55)\varepsilon| + \varepsilon^2$$

Quadratic Example



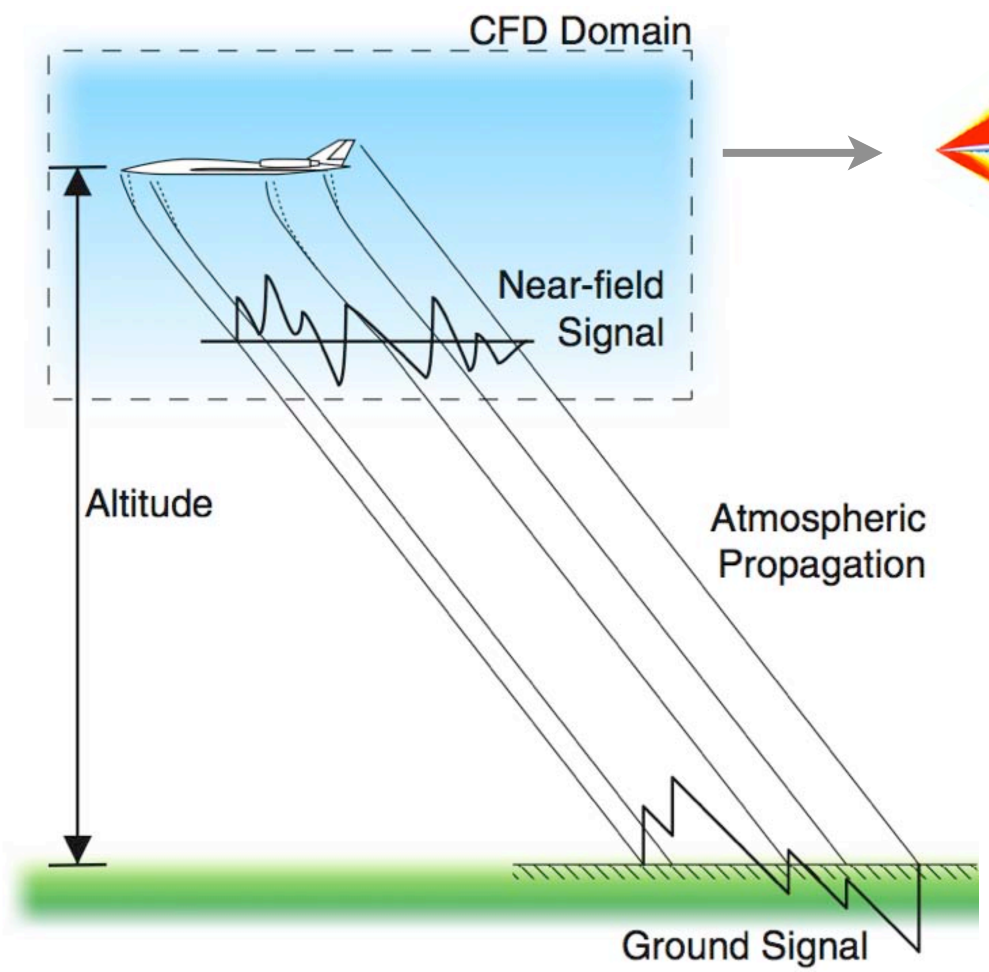
- Objective function error estimate smoothly decreasing in all design cycles

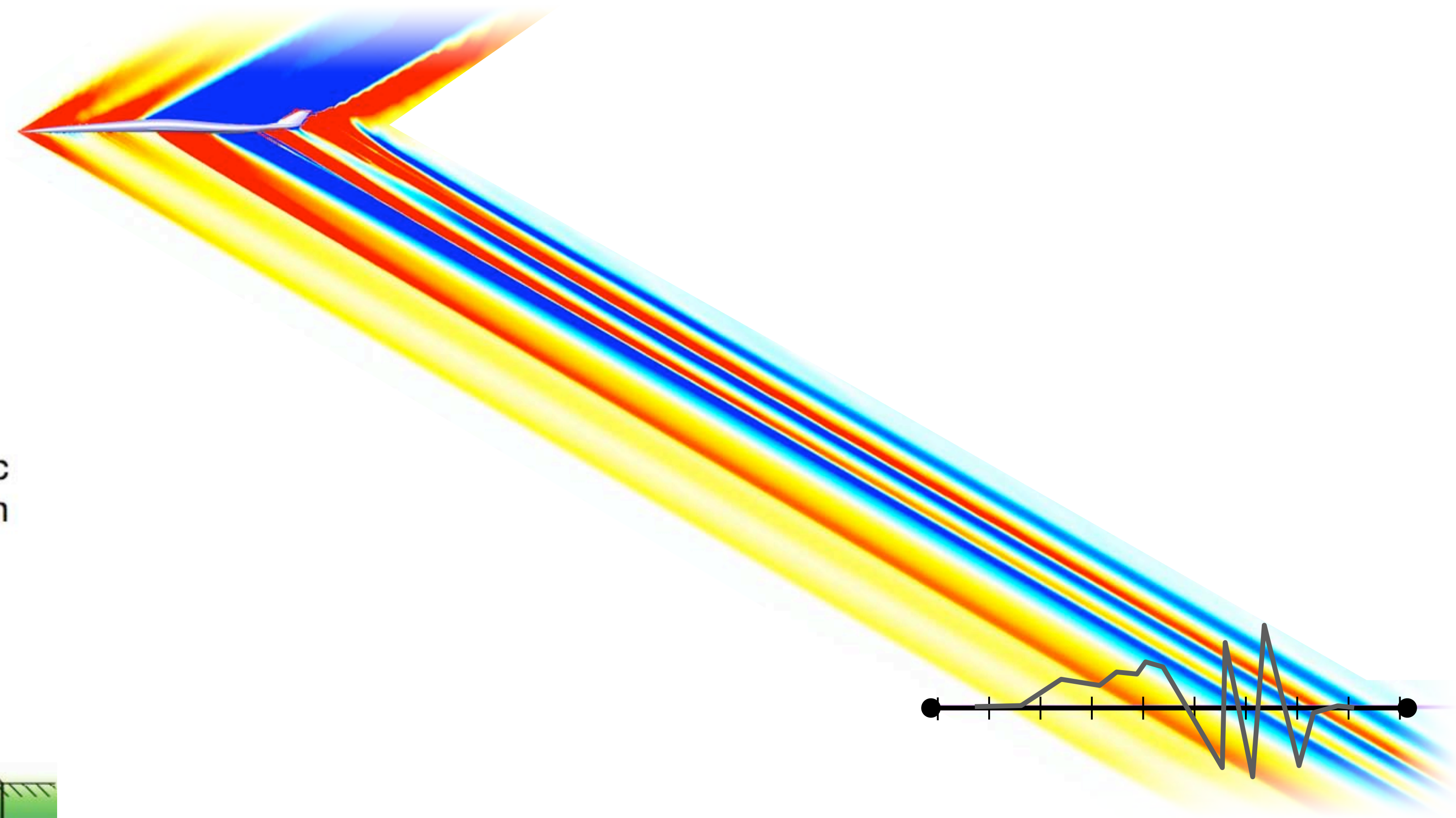
- Eliminated numerical artifact of vanishing error estimate near optimality



Sonic-Boom Mitigation

Drive vehicle shape by prescribing quieter near-field signals

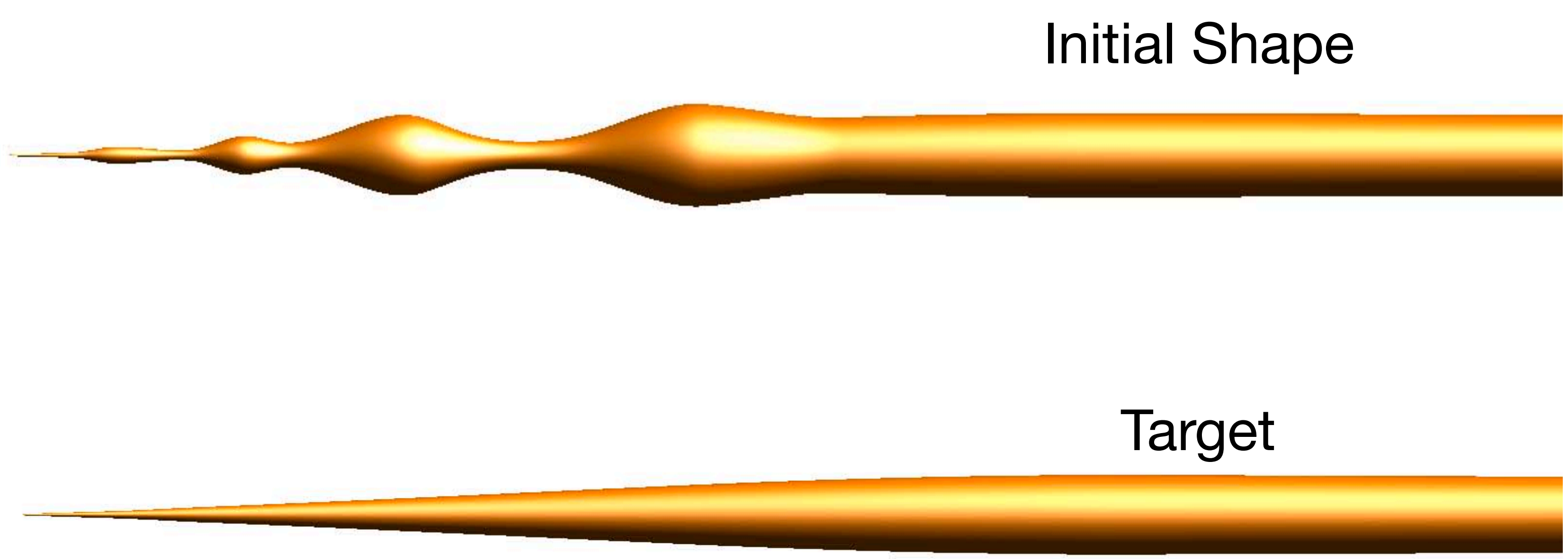


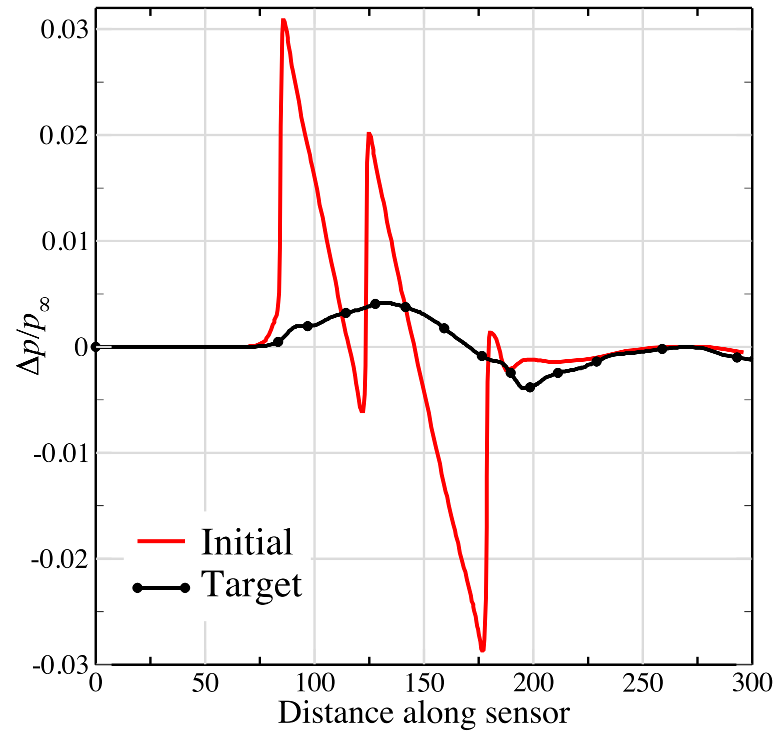


Inverse Design Model Problem

Problem Setup

- Prescribe a target signature from a known shape and verify that the optimization can recover this solution
- 10 design variables that control body radius
- $M_\infty = 1.5$ and $\alpha = 0°$





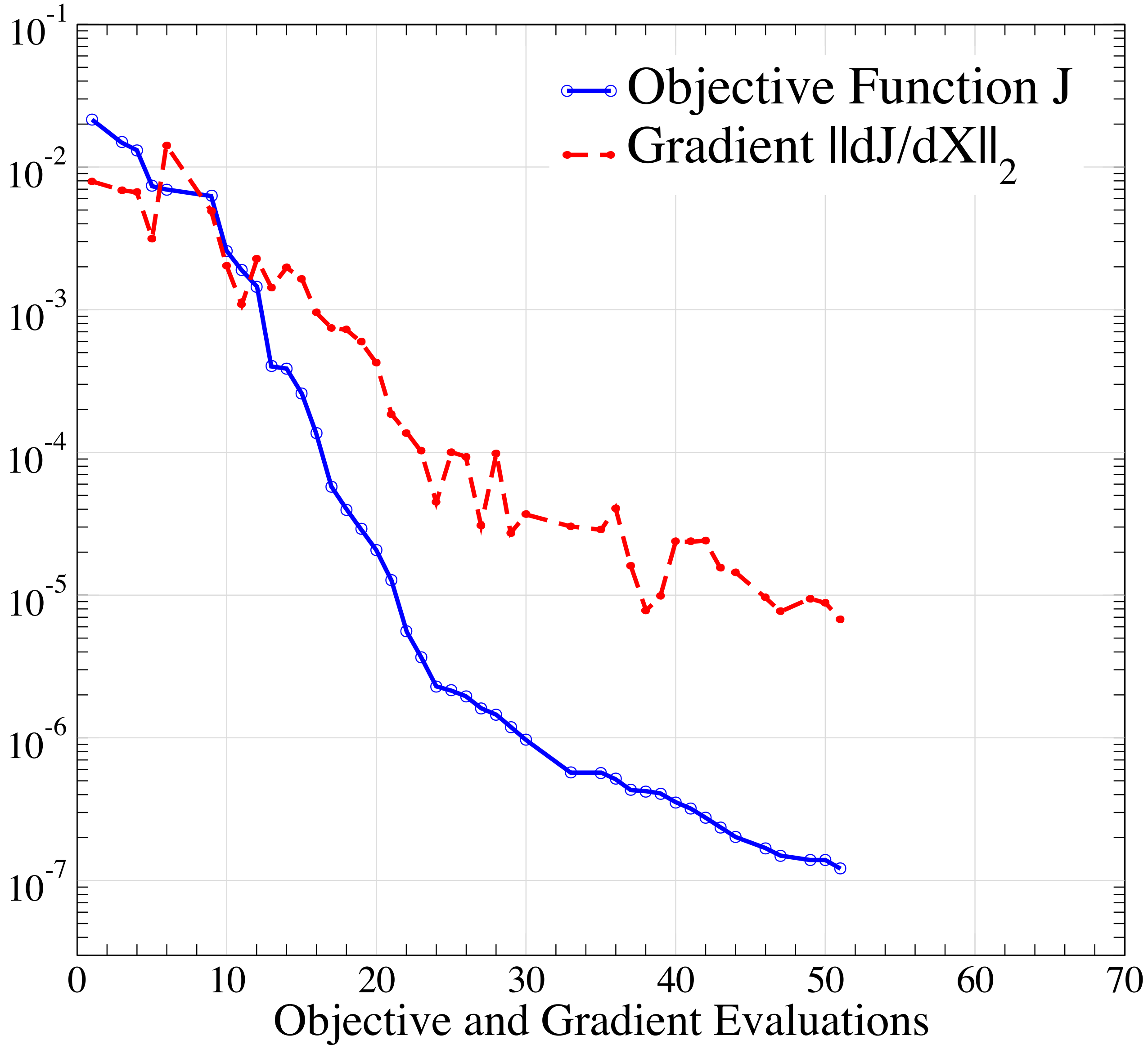
Inverse Design Model Problem

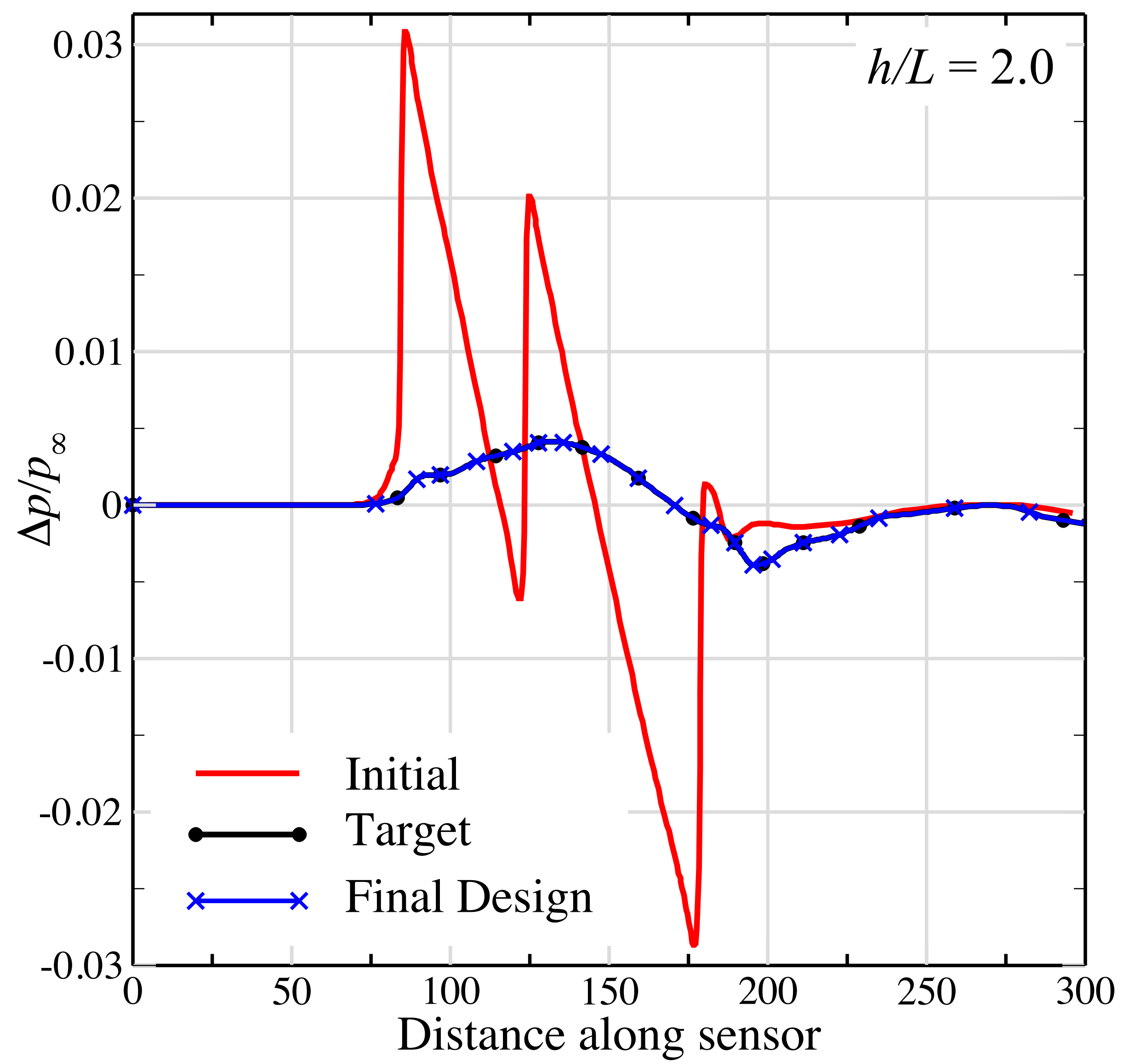
Problem Setup

- Inverse design formulation: $$J = \frac{1}{p_\infty^2} \int (p - p_{\text{target}})^2 dS$$ at h/L = 2
- Error control functional: $$J_{\text{EC}} = \frac{1}{p_\infty^2} \int (p - p_\infty)^2 dS$$
- Consider two cases
  1. Fixed-depth strategy: 7 adaptation cycles in each design iteration
  2. Progressive optimization

Inverse Design Model Problem

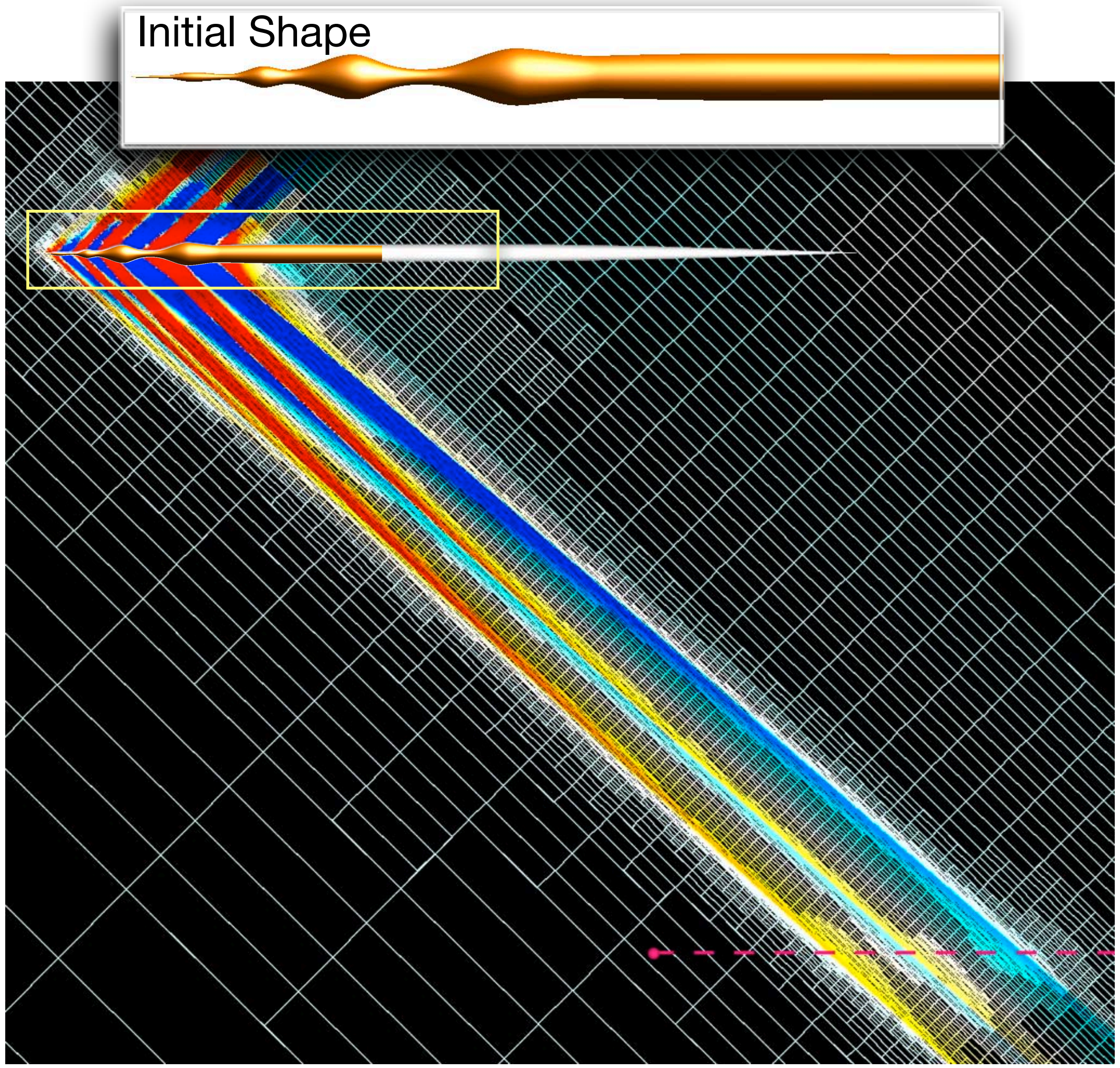
Fixed-Depth Strategy

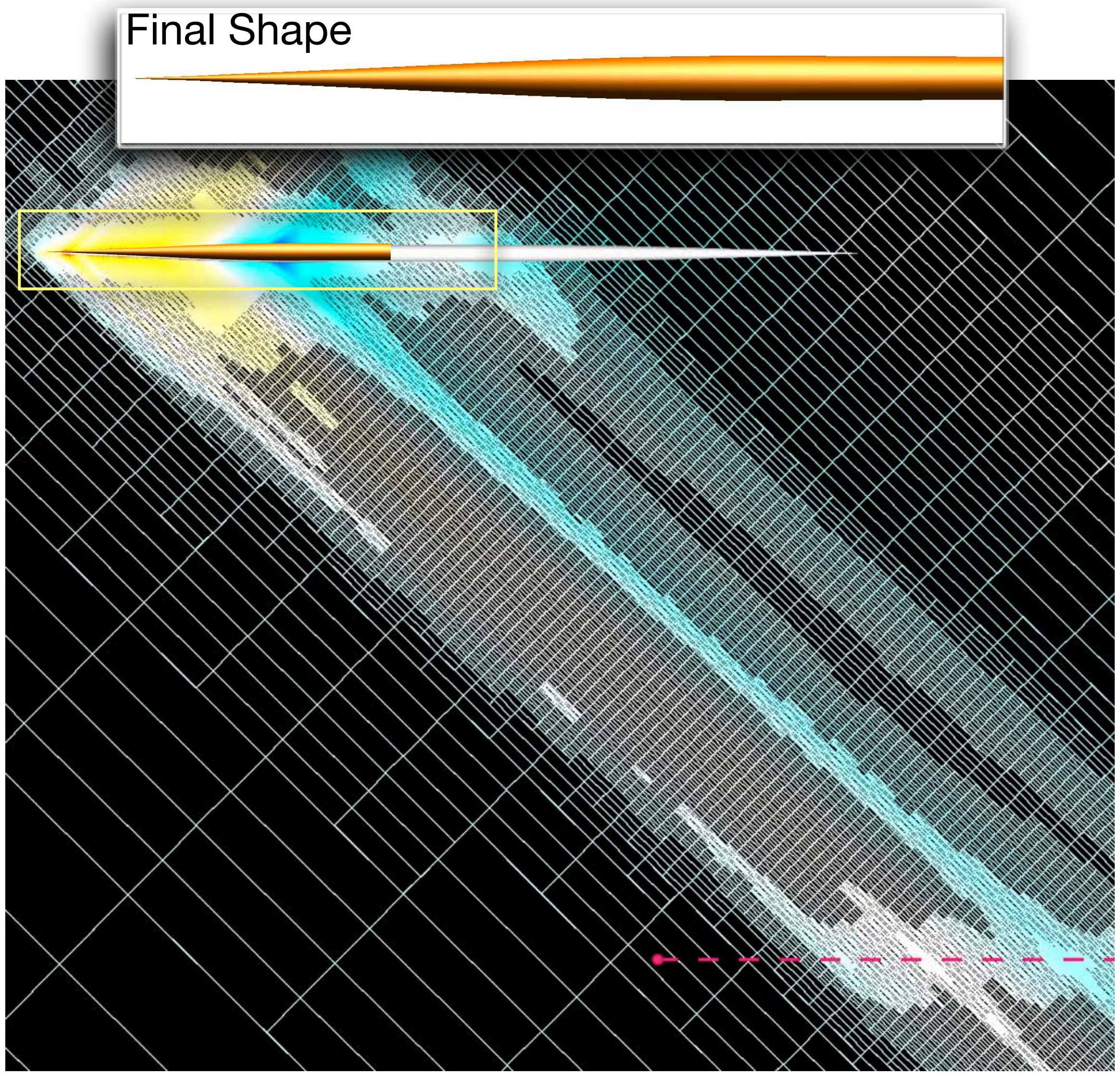




Inverse Design Model Problem

Fixed-Depth Strategy

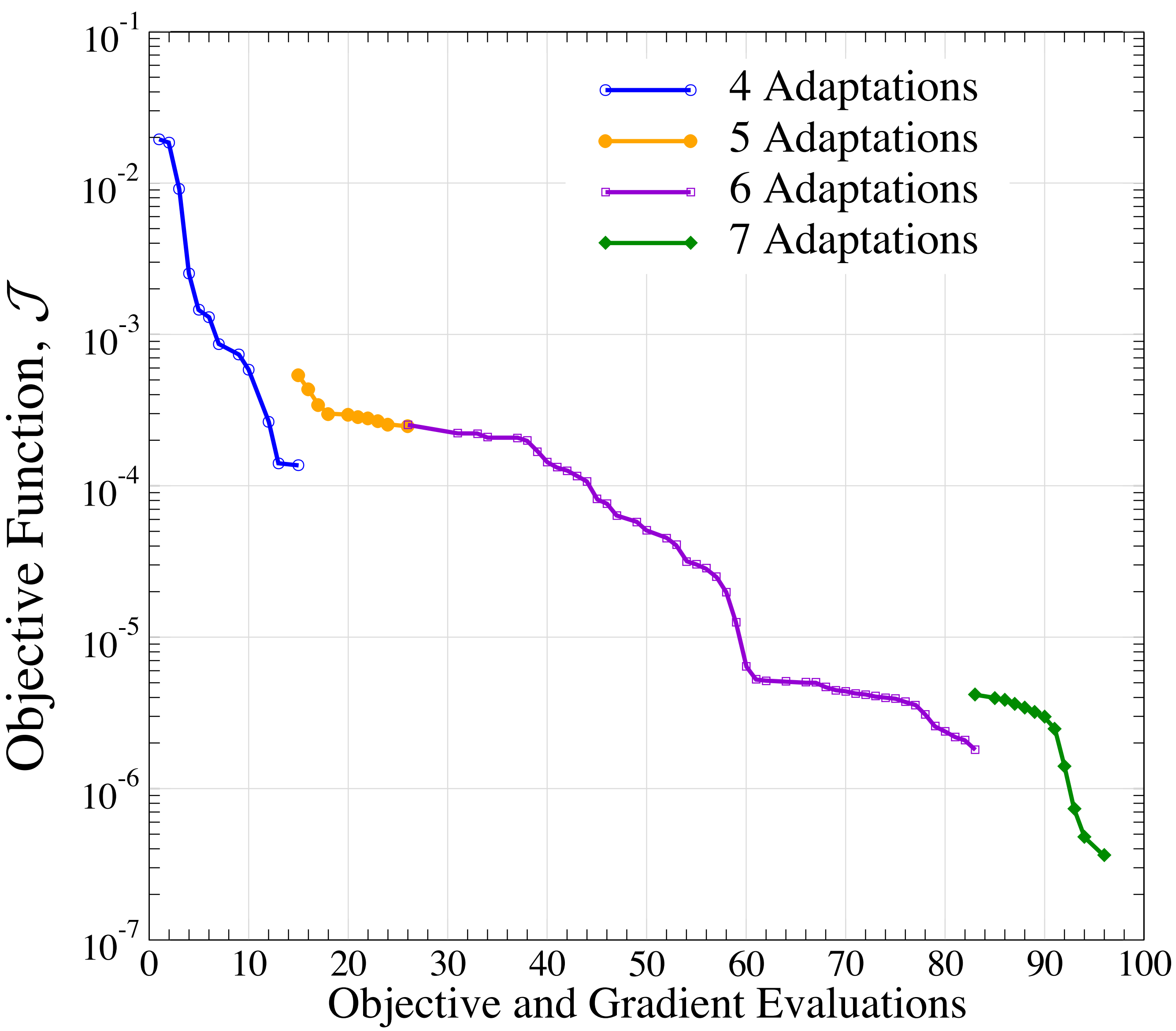


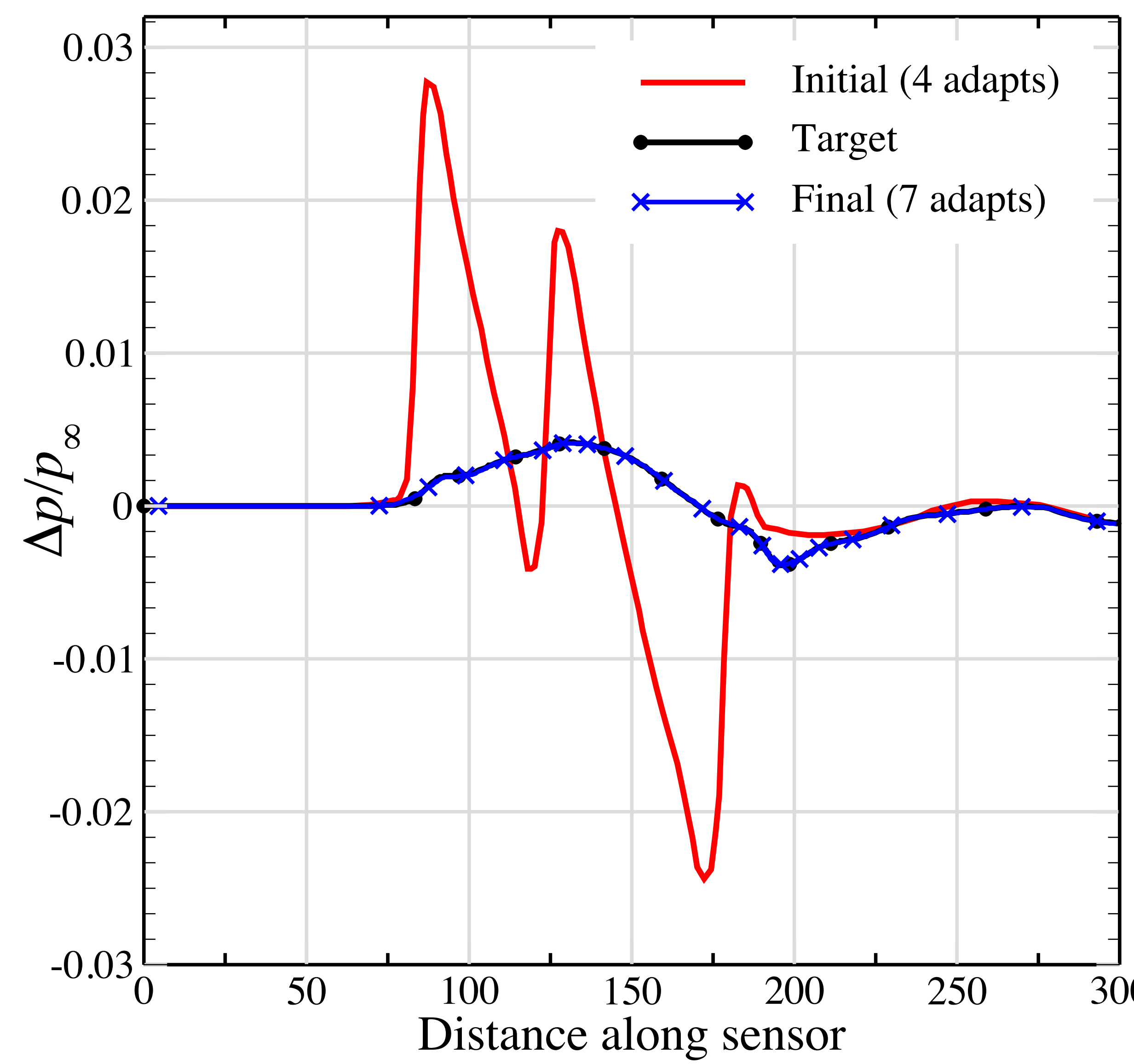


7 Adaptations, ~650k cells

Progressive Optimization

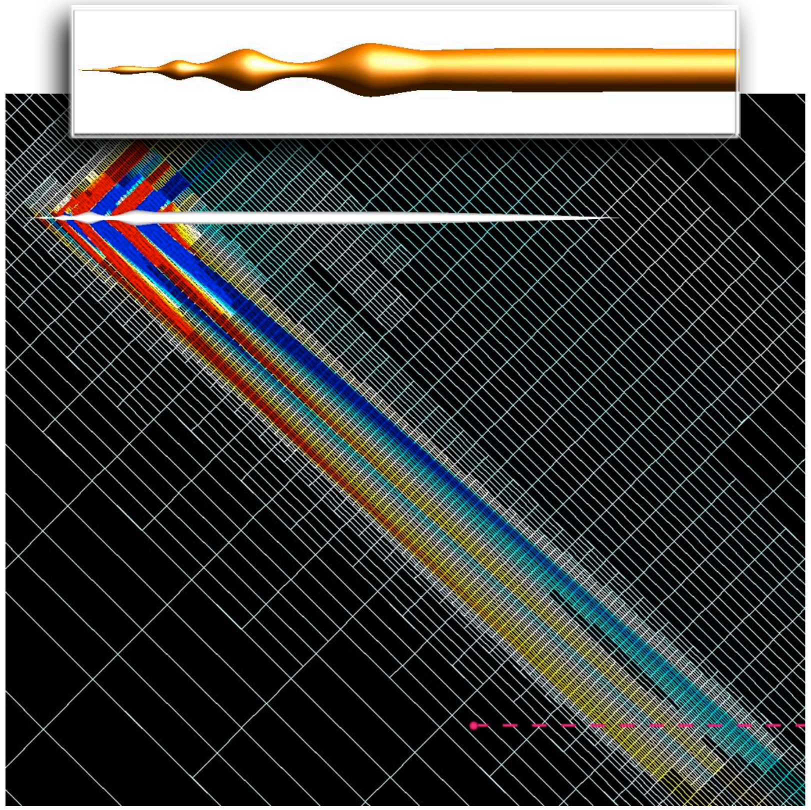
- Minimize number of design iterations performed on finest mesh
- Allow the designs to advance as far as possible on each level



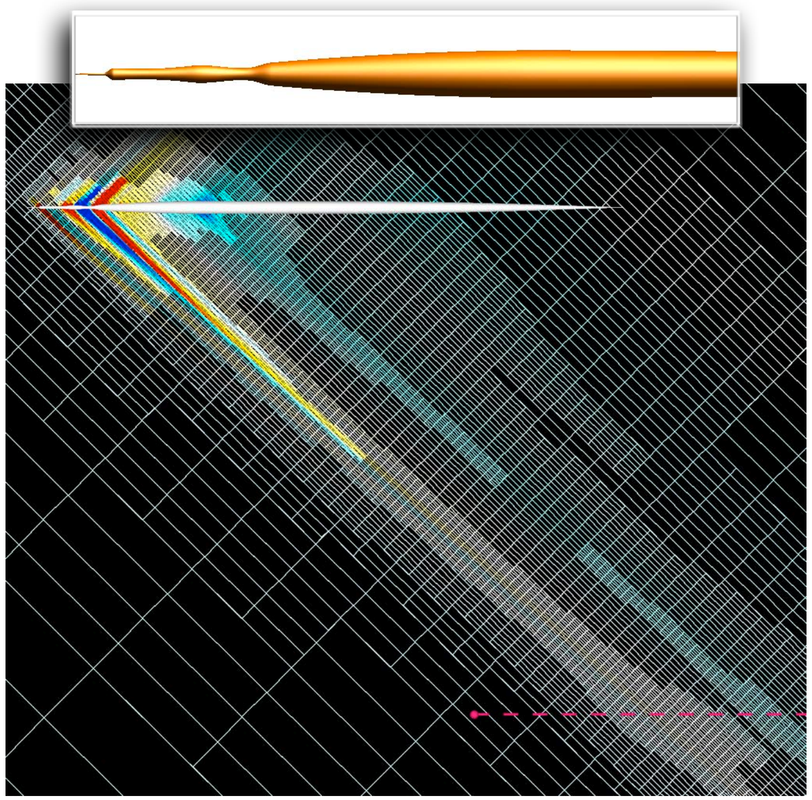


Progressive Optimization

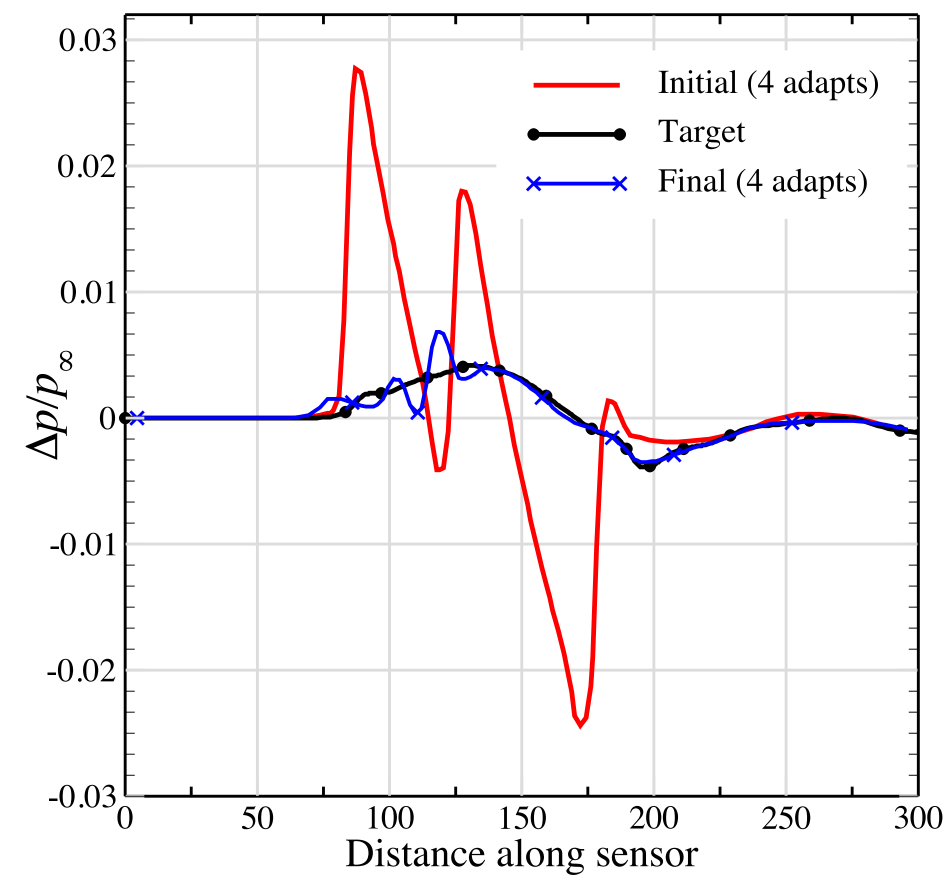
4 Adaptations, ~130k cells



Initial, 4 Adaptations



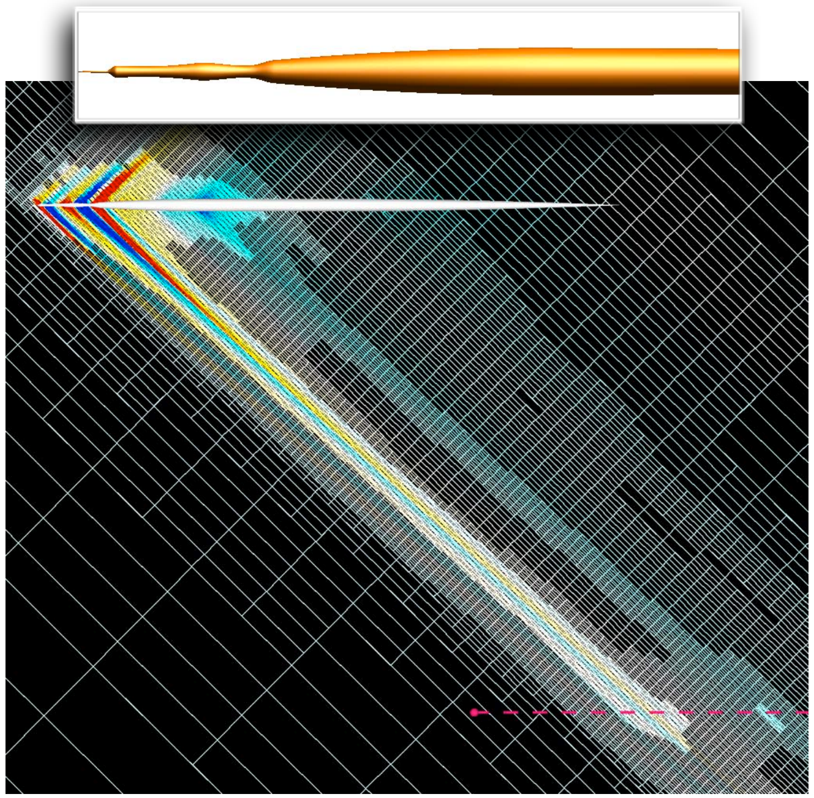
Final, 4 Adaptations



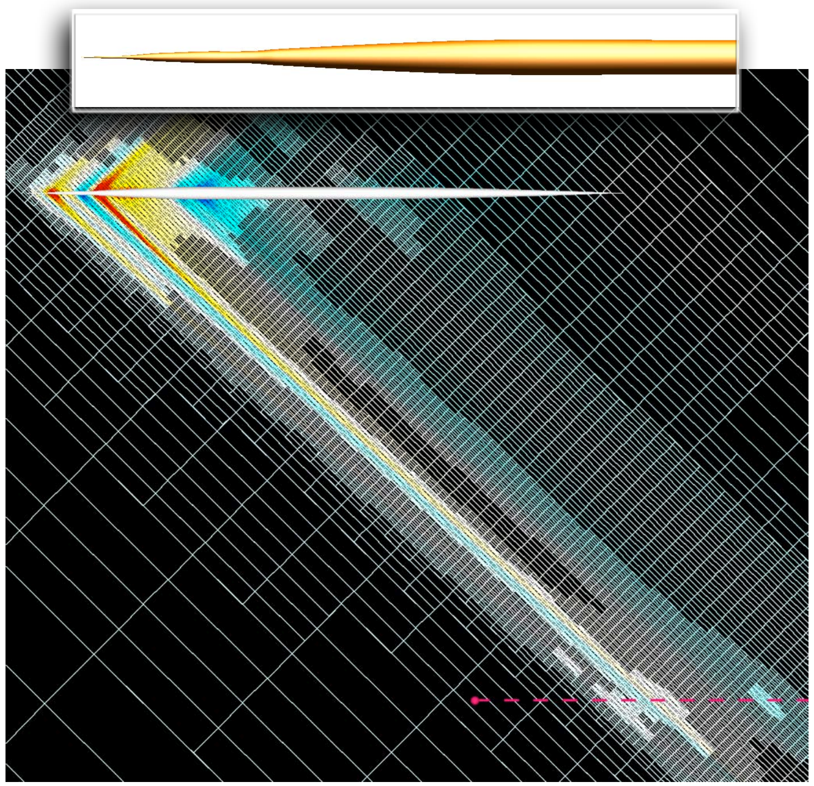
- Terminated due to design variable bound violation near nose
- Peak-to-peak signal reduced by over a factor of five, smooth aft body

Progressive Optimization

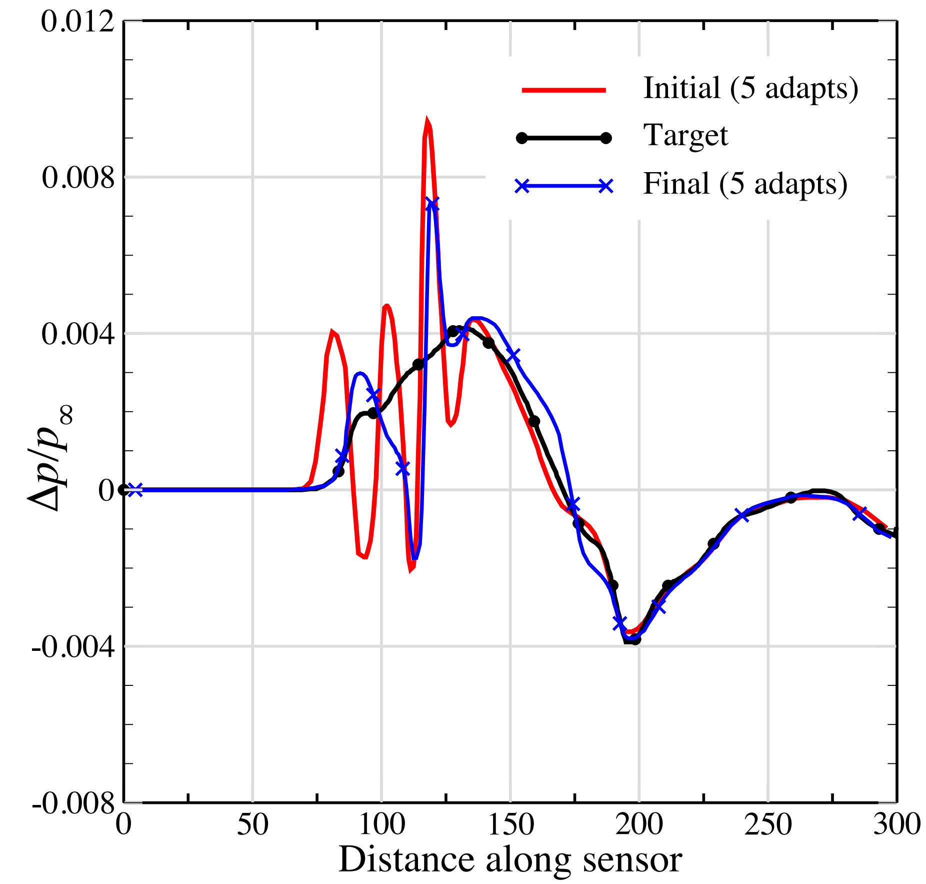
5 Adaptations, ~230k cells



Initial, 5 Adaptations



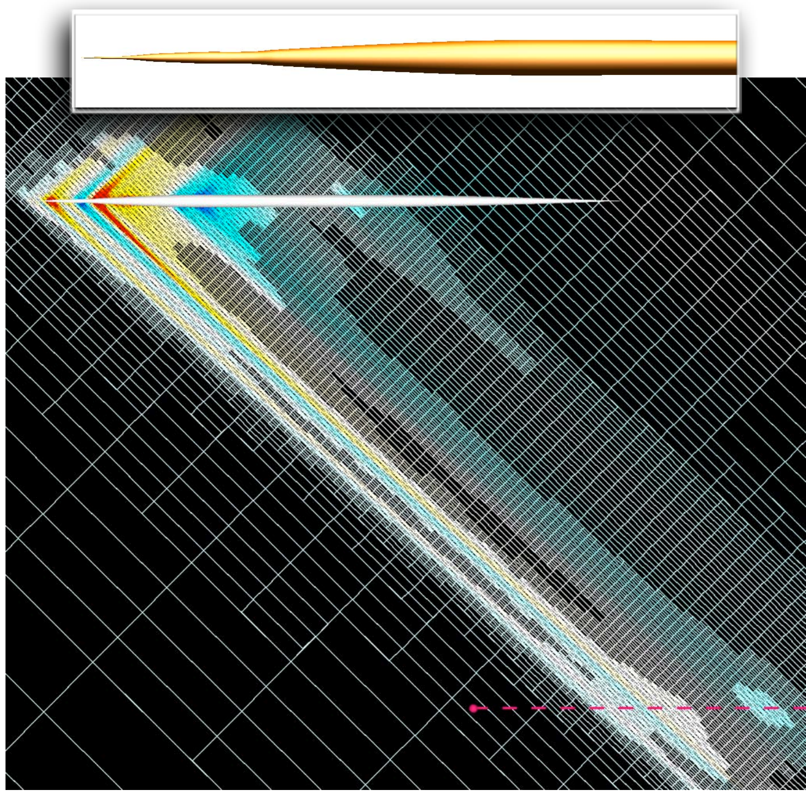
Final, 5 Adaptations



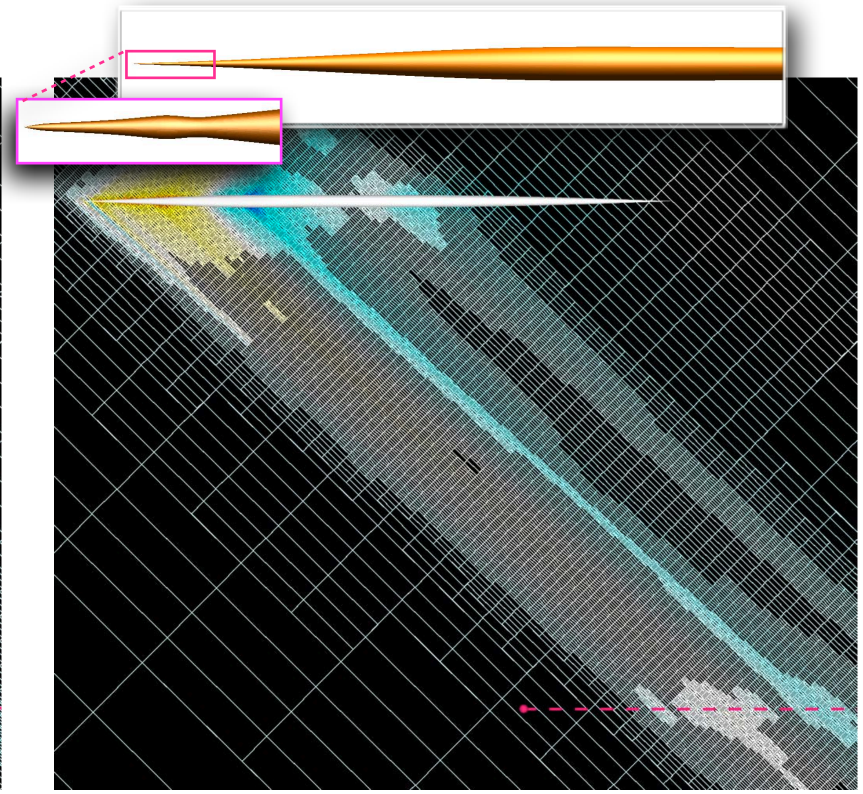
- Terminated due to design variable bound violation near nose
- Smoother nose shape, finer scales not resolvable on the previous mesh

Progressive Optimization

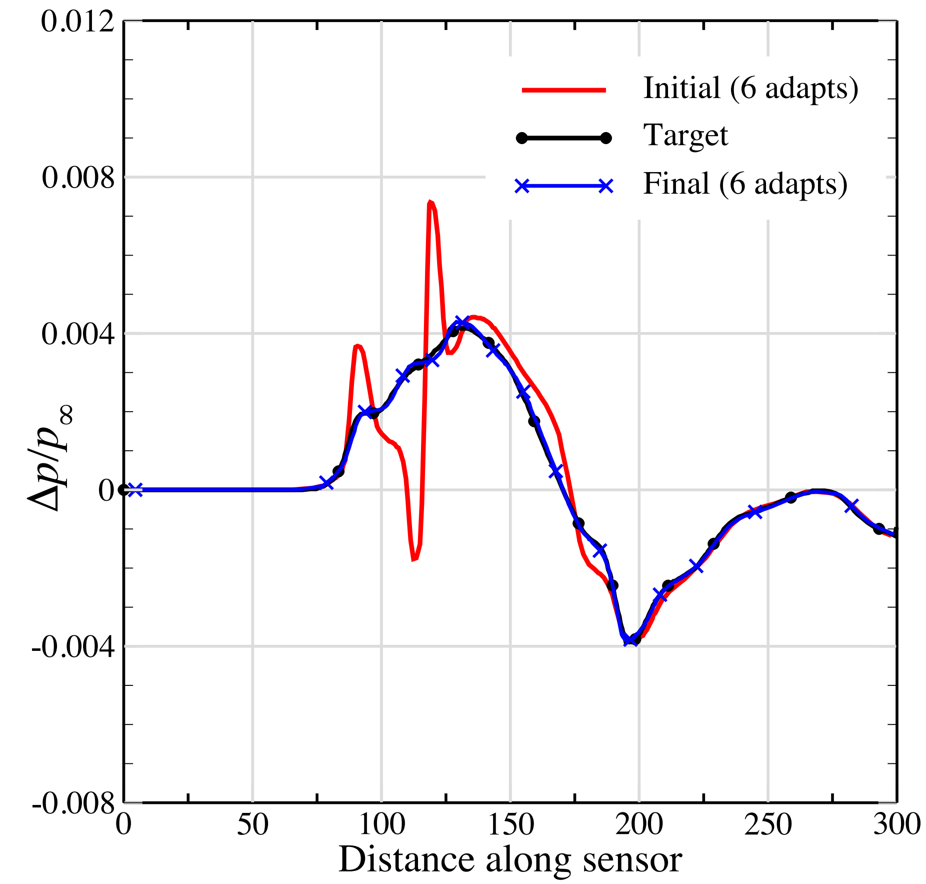
6 Adaptations, ~350k cells



Initial, 6 Adaptations



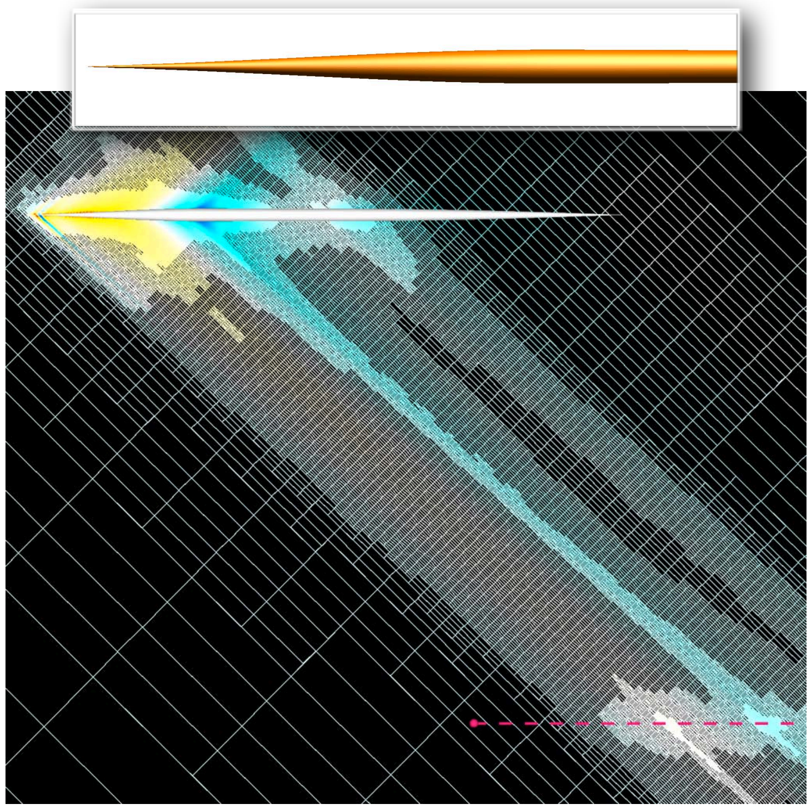
Final, 6 Adaptations



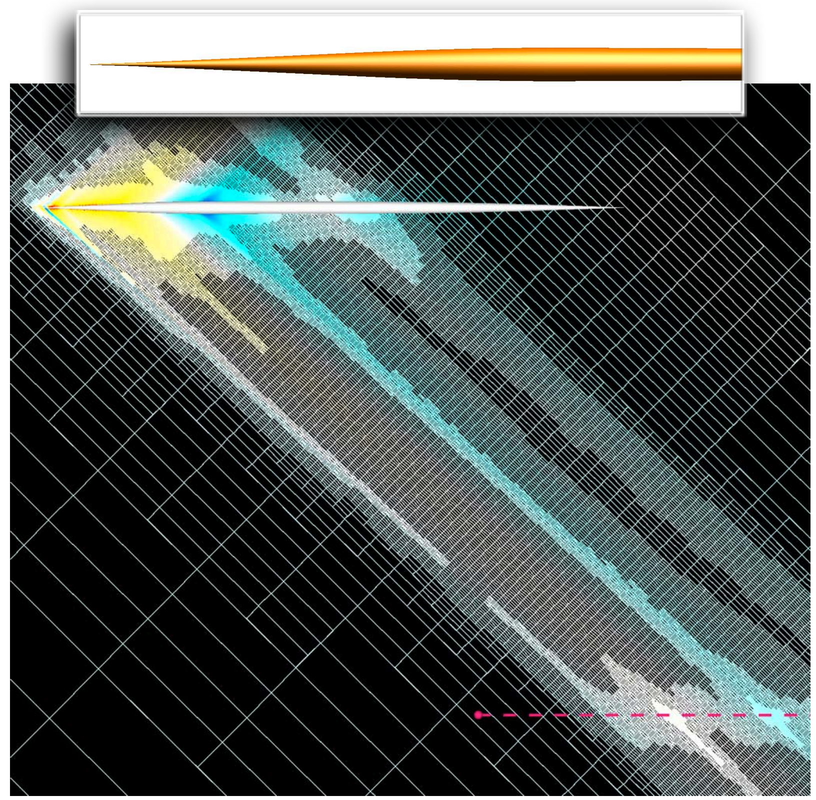
- Most work performed on this mesh: cost is roughly half of fixed-depth example per design iteration
- Target matched to plotting accuracy but tip shape different from target

Sonic-Boom Inverse Design

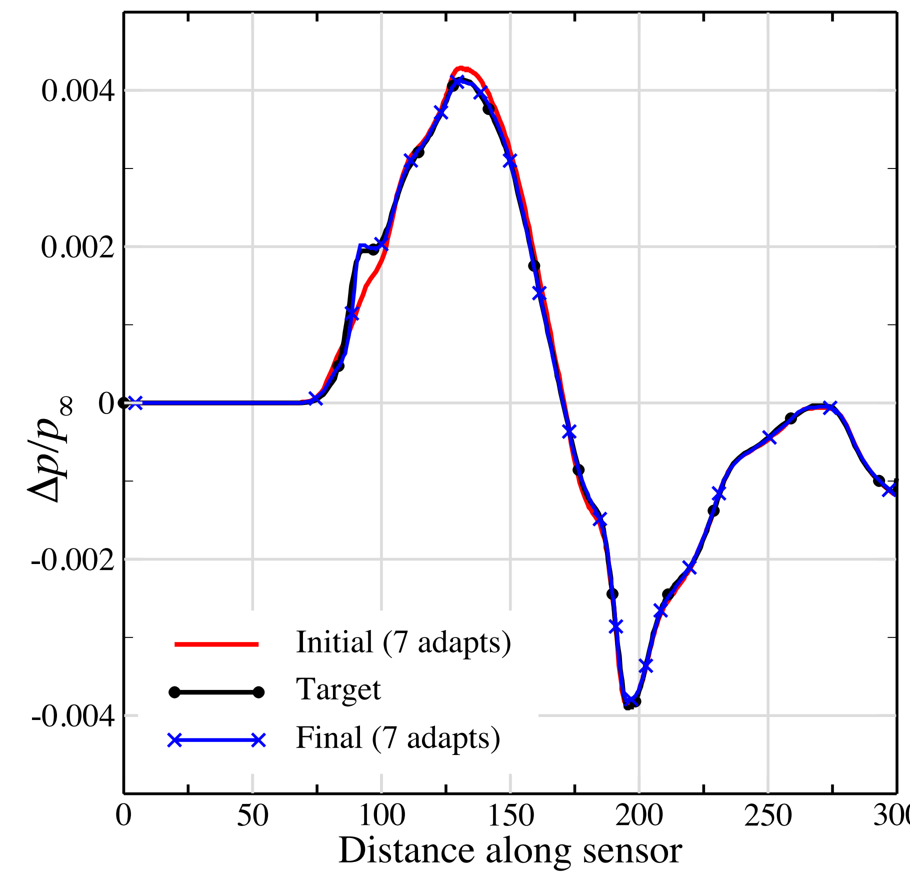
7 Adaptations, ~650k cells



Initial, 7 Adaptations



Final, 7 Adaptations



- Matched target shape in 12 design iterations
- Roughly a factor of two faster than fixed-depth strategy
- Mesh largely unchanged, could we re-use the same mesh?

Summary and Future Work

- Developed framework for gradient-based optimization with capability to perform adaptive meshing in each design iteration
  - Promising approach to enhance accuracy, efficiency and automation of simulation-based design
- Preliminary investigation of dynamic error control
  - Eliminated numerical artifacts in error estimates for objective functions in quadratic form
- Future work
  - Use of error estimates to limit oversolving
  - Transfer of Hessian matrix as the design moves from mesh to mesh
  - Mesh re-use from nearby designs

Questions

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